

Appendix 8.1

Emissions Modeling (TSD Chapter 2)

2.0 EMISSIONS MODELING

2.1 Emissions Modeling Overview

For the emissions modeling work conducted in support of CENRAP air quality modeling, we used updated 2002 emissions data for the U.S., 1999 emissions data for Mexico, and 2000 emissions data for Canada to generate a final base 2002 Base G Typical (Typ02G) annual emissions database. Numerous iterations of the emissions modeling were conducted using interim databases before arriving at the final Base G emission inventories. The 2002 and 2018 emissions inventories and ancillary modeling data were provided by CENRAP emissions inventory contractors (Pechan and CEP, 2005c,e; Reid et al., 2004a,b; Coe and Reid, 2003), other Regional Planning Organizations (RPOs) and EPA. Building from the CENRAP preliminary 2002 database (Pechan and CEP, 2005e) and 2018 projections (Pechan, 2005d), we integrated several updates to the inventories and ancillary data to create final emissions input files; the final simulations are referred to as 2002 Typical and 2018 Base G, or Typ02G and Base18G. We used the Sparse Matrix Operator Kernel Emissions (SMOKE) version 2.1 processing system (CEP, 2004) to prepare the inventories for input to the air quality modeling systems. The SMOKE simulations documented in this report include emissions generated for annual CMAQ and CAMx simulations at a 36-km model grid resolution, and a short-term CMAQ test simulation at a 12-km model grid resolution. We performed the modeling and quality assurance (QA) work based on the CENRAP modeling Quality Assurance Project Plan (QAPP; Morris and Tonnesen, 2004) and Modeling Protocol (Morris et al., 2004a).

The Typ02G and Base18G emission inventories represent significant improvements to the preliminary emissions modeling performed by CENRAP (Morris et al., 2005). While the preliminary 2002 modeling served its purpose to develop the infrastructure for modeling large emissions data sets and producing annual emissions simulations, much of the input data (both as inventories and ancillary data) were placeholders for actual 2002 data that were being prepared through calendar year 2005. As these actual 2002 data sets became available, they were integrated into the SMOKE modeling and QA system that was developed during the preliminary modeling, to produce a high-quality emissions data set for use in the final CMAQ and CAMx modeling. The addition of entirely new inventory categories, like marine shipping, added complexity to the modeling. By the end of the emissions data collection phase, there were 23 separate emissions processing streams covering a variety of sources categories necessary to general model-ready emission inputs for the 2002 calendar year.

2.1.1 SMOKE Emissions Modeling System Background

The purpose of SMOKE (or any emissions processor) is to process the raw emissions reported by states and EPA into gridded hourly speciated emissions required by the air quality model. Emission inventories are typically available as an annual total emissions value for each emissions source, or perhaps with an average-day emissions value. The air quality models, however, typically require emissions data on an hourly basis, for each model grid cell (and perhaps model layer), and for each model species. Consequently, emissions processing involves (at a minimum) transformation of emission inventory data by temporal allocation, chemical speciation, spatial allocation, and perhaps layer assignment, to achieve the input requirements of the air quality model. For the CENRAP modeling effort, all of these steps were needed. In

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addition, CENRAP processing requires special MOBILE6 processing and growth and control of emissions for the future-year inventories. Finally, the biogenic emission processing using BEIS2 includes additional processing steps. SMOKE formulates emissions modeling in terms of sparse matrix operations. Figure 2-1 shows an example of how the matrix approach organizes the emissions processing steps for anthropogenic emissions, with the final step that creates the model-ready emissions being the merging of all the different processing streams of emissions into a total emissions input file for the air quality model. Figure 2-1 does not include all the potential processing steps, which can be different for each source category in SMOKE, but does include the major processing steps listed in the previous paragraph, except the layer assignment. Specifically, the inventory emissions are arranged as a vector of emissions, with associated vectors that include characteristics about the sources such as its state and county or source classification code (SCC). SMOKE also creates matrices that will apply the gridding, speciation, and temporal factors to the vector of emissions. In many cases, these matrices are independent from one another, and can therefore be generated in parallel. The processing approach ends with the merge step, which combines the inventory emissions vector (now an hourly inventory file) with the control, speciation, and gridding matrices to create model-ready emissions.

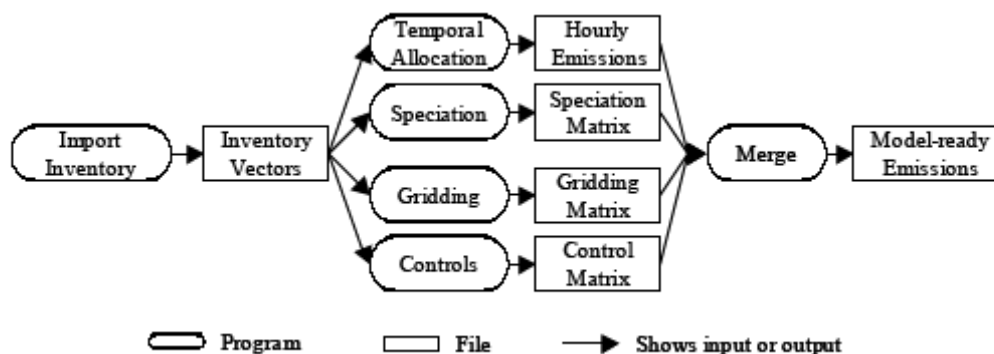


Figure 2-1. Flow diagram of major SMOKE processing steps needed by all source categories.

Temporal processing includes both seasonal or monthly adjustments and day-of-week adjustments. Emissions are known to be quite different for a typical weekday versus a typical Saturday or Sunday. For the day-of-week temporal processing step, emissions may be processed using representative Monday, weekday, Saturday, and Sunday for each month; we refer to this type of processing here as MWSS processing (note that because SMOKE operates in Greenwich Mean Time [GMT] then Monday would include some of local time Sunday so needs to be processed separately from the typical weekday). This approach significantly reduces the number of times the temporal processing step must be run. In the sections below, we have identified the cases in which we have used the MWSS processing approach. Figure 2-2 provides a schematic diagram of SMOKE/BEIS2 processing steps used in this project to generate biogenic emissions rates for Volatile Organic Compounds (VOCs) and oxides of nitrogen (NO_x). Because biogenic emissions are temperature sensitive, they are generated for each day of 2002 using day-specific meteorological conditions from the MM5 meteorological model.

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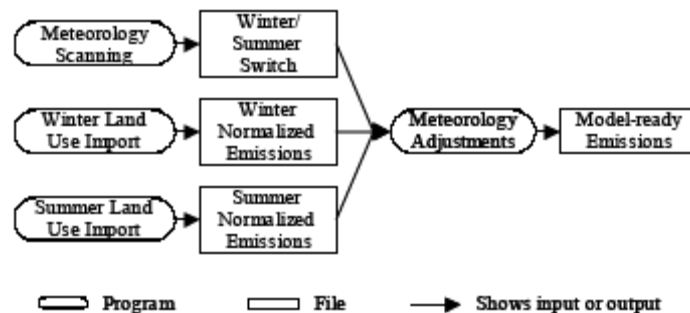


Figure 2-2. Flow diagram of SMOKE/BEIS2 processing steps.

2.1.2 SMOKE Scripts

The scripts are the interface that emissions modelers use to run SMOKE and define the set up and databases used in the emissions modeling so are important for anyone wishing to reproduce the CENRAP SMOKE emissions modeling. Many iterations of the CENRAP SMOKE emissions modeling were performed using updated and corrected emissions data and assumptions resulting in the creation of numerous SMOKE modeling scripts during the course of the study. For the CENRAP annual 2002 SMOKE emissions modeling, the default SMOKE script set up, which is based on source categories, was used to configure the scripts. We made several modifications to the default SMOKE scripts to modularize them, add error checking loops, and break up the report and logs directories by source category. The result is one script for each major source category being modeled that calls all of the SMOKE programs required for simulating that source category. 16 major source categories were modeled by SMOKE for CENRAP. An addition seven SMOKE scripts were also run to set up the emissions modeling. Table 2-1 lists all of the SMOKE scripts used for the 2002 base year modeling and the SMOKE programs called by each script. In addition to the source-specific scripts listed in Table 2-1, we also listed the SMOKE utility scripts that actually call executables, manage the log files, and manage the configuration of the SMOKE simulations.

Table 2-1. Summary of SMOKE scripts

Source Category	Script Name	SMOKE Programs/Functions
Area	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_ar_base02f.csh	smkinev, grdmat, spcmat, temporal, smkmerge, smkreport
Area fire	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_arf_base02f.csh	smkinev, grdmat, spcmat, temporal, smkmerge, smkreport
Offshore Area	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_ofsar_base02f.csh	smkinev, grdmat, spcmat, temporal, smkmerge, smkreport
Non-road [*]	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_nr_base02f.csh	smkinev, grdmat, spcmat, temporal, smkmerge, smkreport
Mobile	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_fd_base02f.csh	smkinev, grdmat, spcmat, temporal, smkmerge, smkreport
Fugitive dust	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_rd_base02f.csh	smkinev, grdmat, spcmat, temporal, smkmerge, smkreport
Road dust	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_nh3_base02f.csh	smkinev, grdmat, spcmat, temporal, smkmerge, smkreport
Ammonia [*]	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_mb_base02f.csh	smkinev, grdmat, spcmat, temporal, smkmerge, smkreport
On-road	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_nusm_base02f.csh	smkinev, grdmat, spcmat, temporal, smkmerge, smkreport
Mobile (non-VMT-based)	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_mbv_base02f.csh	smkinev, grdmat, spcmat, temporal, smkmerge, smkreport
On-road non-US Mobile (non-VMT-based)	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_mbssetup_base02f.csh	smkinev, mbssetup, grdmat, spcmat, premobl, emisfac, temporal, smkmerge, smkreport
On-road Mobile (VMT-based)	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_wog_base02f.csh	smkinev, grdmat, spcmat, temporal, smkmerge, smkreport
WRAP Oil and Gas	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_pt_base02f.csh	smkinev, grdmat, spcmat, laypoint, temporal, smkmerge, smkreport
Point	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_ofs_base02f.csh	smkinev, grdmat, spcmat, laypoint, temporal, smkmerge, smkreport
Offshore point	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_bsfc_base02f.csh	smkinev, grdmat, spcmat, laypoint, temporal, smkmerge, smkreport
Canadian Point fires	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_alf_base02f.csh	smkinev, grdmat, spcmat, laypoint, temporal, smkmerge, smkreport
All point fires	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_bg_base02f.csh	smkinev, grdmat, spcmat, laypoint, temporal, smkmerge, smkreport
Biogenec	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_run.csh	Normbies3, tmbpies3, smkmerge
n/a	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/make_inmdir.csh	builds output file names and directories
n/a	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/smk_run.csh	Calls SMOKE executables for everything but projection, controls, and QA
n/a	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/qa_run.csh	Calls the SMOKE executables for running QA program & names the input/output directories for reports
n/a	/home/aqm2/edss2/cenrap02f/subsys/smoke/scripts/run/36km/smk_calls.csh	Calls smk_run.csh, qa_run.csh, configuration and management
n/a	/home/aqm2/edss2/cenrap02f/subsys/smoke/Assignes/ASSIGNES.cenrap_base02f.cmaq.cb4 p25	Sets up the environment variables for use of SMOKE
n/a	/home/aqm2/edss2/cenrap02f/subsys/smoke/Assignes/smk_mkdir	Creates the input/output directories
n/a	/home/aqm2/edss2/cenrap02f/subsys/smoke/Assignes/setmerge_files.scr	Sets up the output environment variables for the smkmerge program

^{*} The nr and nh3 where farther divided to nrm and nry and nh3m and nh3y for the monthly/seasonal and yearly inventories

2.1.3 SMOKE Directory Structures

The SMOKE directories can be divided into three broad categories:

1. Program Directories: These directories contain the model source code, assigns files, scripts and executables needed to run SMOKE.
2. Input Directories: These directories contain the raw emissions inventories, the meteorological data and the ancillary input files.
3. Output Directories: These directories contain all of the output from the model. Also, the output directories contain the MOBILE6 input files.

The directories are described in the Table 2-2. The final pre-merged emission file names and sources of the data re provided in Appendix B.

Table 2-2. Summary of SMOKE directories.

Category	Directory Location	Directory Contents
Program	/home/aqm2/edss2/ cenrap02f/subsys/smoke/src	SMOKE source code
	/home/aqm2/edss2/ cenrap02f/subsys/smoke/assigns	SMOKE assigns files
	/home/aqm2/edss2/ cenrap02f/subsys/smoke/scripts	SMOKE make and run scripts
	/home/aqm2/edss2/ cenrap02f/subsys/smoke/Linux2_x86pg	SMOKE executables
Input	/home/aqm2/edss2/ cenrap02f/data/met	MCIP out metrology files
	/home/aqm2/edss2/ cenrap02f/data/ge_dat	SMOKE ancillary input files
	/home/aqm2/edss2/ cenrap02f/data/inventory/cenrap2002	Raw emissions inventory files
Output	/home/aqm2/edss2/ cenrap02f/data/run_base02f/static	Non-time dependent SMOKE intermediate outputs and MOBILE6 inputs
	/home/aqm2/edss2/ cenrap02f/data/run_base02f/scenario	Time dependent SMOKE intermediate outputs
	/home/aqm2/edss2/ cenrap02f/data/run_base02f/outputs	Model-ready SMOKE outputs
	/home/aqm2/edss2/ cenrap02f/data/reports	SMOKE QA reports

2.1.3 SMOKE Configuration

SMOKE was configured to generate emissions for all months of 2002 on the 36-km unified RPO modeling domain (Figure 1-2). For the anthropogenic emissions sources that use hourly meteorology and daily or hourly data (i.e., on-road mobile sources, point sources with CEM data, point source fires and biogenic sources) we configured SMOKE to represent the daily emissions explicitly. For the non-meteorology dependent emissions, we used a representative Saturday, Sunday, Monday, and weekday for each month as surrogate days for the entire month's emissions (we refer to this as the MWSS processing approach). For these non-meteorology dependent emissions sources we explicitly represented the holidays as Sundays. Table 2-3 lists the days that we modeled as representative days in the months that we simulated for the 2002 base year modeling. Table 2-4 lists the holidays in 2002 that were modeled as Sundays.

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Table 2-3: Representative model days for 2002 base year simulation.

Saturday	Sunday	Monday	Weekday
January 5	January 6	January 7	January 4
February 2	February 3	February 4	February 5
March 2	March 3	March 4	March 5
April 6	April 7	April 8	April 2
May 4	May 5	May 6	May 7
June 8	June 9	June 3	June 4
July 6	July 7	July 8	July 3
August 3	August 4	August 5	August 6
September 7	September 8	September 9	September 10
October 5	October 6	October 7	October 8
November 2	November 3	November 4	November 5
December 7	December 8	December 9	December 10

Table 2-4: 2002 modeled holidays.

Holiday	Date
New Years	January 1, 2002 January 2, 2002
Good Friday	March 29, 2002 March 30, 2002
Memorial Day	May 27, 2002 May 28, 2002
Independence Day	July 4, 2002 July 5, 2002
Labor Day	September 2, 2002 September 3, 2002
Thanksgiving Holiday	November 28-30, 2002
Christmas Holiday	December 24-26, 2002

We used the designations in Table 2-5 to determine which months fell into each season when temporally allocating the seasonal emissions inventories. Some of the inventories for the Electrical Generating Units (EGUs) were received for Winter and Summer. Table 2-6 determines which months fell into each season

Table 2-5: Assignments of months to four seasons for use of seasonal inventory files in SMOKE.

Month	Season
January	Winter
February	Winter
March	Spring
April	Spring
May	Spring
June	Summer
July	Summer
August	Summer
September	Fall
October	Fall
November	Fall
December	Winter

Table 2-6: Assignments of months to two seasons for use of seasonal inventory files in SMOKE.

Month	Season
January	Winter
February	Winter
March	Winter
April	Winter
May	Summer
June	Summer
July	Summer
August	Summer
September	Summer
October	Winter
November	Winter
December	Winter

2.1.5 SMOKE Processing Categories

Emissions inventories are typically divided into area, on-road mobile, non-road mobile, point, and biogenic source categories. These divisions arise from differing methods for preparing the inventories, different characteristics and attributes of the categories, and how the emissions are processed through models. Generally, emissions inventories are divided into the following source categories, which we refer to later as “SMOKE processing categories.”

- **Stationary Area Sources:** Sources that are treated as being spread over a spatial extent (usually a county or air district) and that are not movable (as compared to non-road mobile and on-road mobile sources). Because it is not possible to collect the emissions at each point of emission, they are estimated over larger regions. Examples of stationary

area sources are residential heating and architectural coatings. Numerous sources, such as dry cleaning facilities, may be treated either as stationary area sources or as point sources.

- On-Road Mobile Sources: Vehicular sources that travel on roadways. These sources can be computed either as being spread over a spatial extent or as being assigned to a line location (called a link). Data in on-road inventories can be either emissions or activity data. Activity data consist of vehicle miles traveled (VMT) and, optionally, vehicle speed. Activity data are used when SMOKE will be computing emission factors via another model, such as MOBILE6 (U.S. EPA, 2005). Examples of on-road mobile sources include light-duty gasoline vehicles and heavy-duty diesel vehicles.
- Non-Road Mobile Sources: These sources are engines that do not always travel on roadways. They encompass a wide variety of source types from lawn and garden equipment to locomotives and airplanes. Emission estimates for most non-road sources come from EPA's NONROAD model (OFFROAD in California). The exceptions are emissions for locomotives, airplanes, pleasure craft and commercial marine vessels.
- Point Sources: These are sources that are identified by point locations, typically because they are regulated and their locations are available in regulatory reports. In addition, elevated point sources will have their emissions allocated vertically through the model layers, as opposed to being emitted into only the first model layer. Point sources are often further subdivided into electric generating unit (EGU) sources and non-EGU sources, particularly in criteria inventories in which EGUs are a primary source of NO_x and SO₂. Examples of non-EGU point sources include chemical manufacturers and furniture refinishers. Point sources are included in both criteria and toxics inventories.
- Biogenic Land Use Data: Biogenic land use data characterize the types of vegetation that exist in either county-total or grid cell values. The biogenic land use data in North America are available using two different sets of land use categories: the Biogenic Emissions Landcover Database (BELD) version 2 (BELD2), and the BELD version 3 (BELD3) (CEP, 2004b).

In addition to these standard SMOKE processing categories, we have added other categories either to represent specific emissions processes more accurately or to integrate emissions data that are not compatible with SMOKE. Examples of emissions sectors that fall outside of the SMOKE processing categories include emissions generated from process-based models for representing windblown dust and agricultural ammonia (NH₃) sources. An emissions category with data that are not compatible with SMOKE is one with gridded emissions data sets, such as commercial marine sources. Another nonstandard emissions category that we modeled was emissions from fires. All of the emissions categories that we used to build CENRAP simulations are described in detail in the following sections.

Continuing the enhancement of the emissions source categories that we initiated during the preliminary 2002 modeling, we further refined the categories from the standard definitions listed above to include more explicit emissions sectors. The advantage of using more detailed definitions of the source categories is that it leads to more flexibility in designing control strategies, substituting new inventory or profile data into the modeling, managing the input and output data from SMOKE and conducting QA of the SMOKE outputs. The major drawback to defining more emissions source categories is the increased level of complexity and computational requirements (run times and disk space) that results from having a larger number of input data sets. Another motivation behind separating the various emissions categories is

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related to the size and flexibility of the input data. Some data sets, like the CENRAP on-road mobile inventory, were so large that we had to process them separately from the rest of the sources in the on-road sector due to computational constraints. We also separated the non-road mobile and ammonia sectors into yearly and monthly inventories to facilitate the application of uniform monthly temporal profiles to the monthly data. Additional details about how we prepared the emissions inventories and ancillary data for modeling are described in Sections 2.2 through 2.16. Table 2-7 summarizes the entire group of source sectors that composed simulation Typ02G. Each emissions sector listed in the table represents an explicit SMOKE simulation. As discussed in Section 2.1.2 below, after finishing all of the source-specific simulations, we used SMOKE to combine all of the data into a single file for each day for input to the air quality modeling systems. Each subsection on the emissions sectors describes each sector in terms of the SMOKE processing category, the year covered by the inventory, and the source(s) of the data. Additional details about the inventories are also provided, including any modifications that we made to prepare them for input into SMOKE.

Table 2-7. CENRAP Typ02G emissions categories.

Emissions Sector	Abbreviation*
Fires as Point Sources (WRAP, CENRAP, VISTAS)	Alf
Area Sources (All domain)	ar
CENRAP area fires	arf
Area fires, Anthropogenic (All domain, excluding WRAP and CENRAP)	arfa
Area fires, Wild (All domain, excluding WRAP)	arfw
Biogenic	b3
Ontario, Canada, point-source fires	bsf
Fugitive dust	fd
WRAP on-road mobile	mb
CENRAP on-road mobile	mbv_CENRAP
Other US on-road mobile	mbv
Monthly CENRAP/MRPO anthropogenic NH ₃	nh3m
Ammonia from annual inventory (CENRAP)	nh3y
WRAP anthropogenic NH ₃	nh3
Seasonal/Monthly non-road mobile (WRAP, CENRAP, MW)	nrm
Annual non-road mobile	nry
On-road Mobile (Non-US)	nusm
Offshore shipping (Gulf, Atlantic)	ofs
Offshore area (Gulf)	ofsar
Stationary point (All domain, including offshore)	pt
Road dust	rd
Windblown dust (All domain)	wb_dust
WRAP oil and gas	wog

*These abbreviations are used in the file naming of the SMOKE output files for each sector.

Emissions models such as SMOKE are computer programs that convert annual or daily estimates of emissions at the state or county level to hourly emissions fluxes on a uniform spatial grid that are formatted for input to an air quality model. For the Typ02G and Base18G emission inventories we prepared emissions for CMAQ version 4.5 using SMOKE version 2.1 on the UCR Linux computing cluster. SMOKE integrates annual county-level emissions inventories with source-based temporal, spatial, and chemical allocation profiles to create hourly emissions fluxes on a predefined model grid. For elevated sources that require allocation of the emissions to the vertical model layers, SMOKE integrates meteorology data to derive dynamic vertical profiles. In addition to its capacity to represent the standard emissions processing categories, SMOKE is also instrumented with the Biogenic Emissions Inventory System, version 3 (BEIS3) model for estimating biogenic emissions fluxes (U.S. EPA, 2004) and the MOBILE6 model for estimating on-road mobile emissions fluxes from county-level vehicle activity data (U.S. EPA, 2005a).

SMOKE uses C-Shell scripts as user interfaces to set configuration options and call executables. SMOKE is designed with flexible QA capabilities to generate standard and custom reports for checking the emissions modeling process. After modeling all of the source categories individually, including those categories generated outside of SMOKE, we used SMOKE to merge all of the categories together to create a single CMAQ input file per simulation day. Also, for use in the CAMx modeling, we converted the CMAQ-ready emissions estimates to CAMx-ready files using the CMAQ2CAMx converter. Additional technical details about the version of SMOKE used for final simulations are available from CEP (2004b). All scripts, data, and executables used to generate the Typ02G and Base18G emissions for CMAQ and CAMx are archived on the CENRAP computing cluster.

2.1.6 2002 and 2018 Data Sources

This section describes the procedures that the CENRAP followed to collect and prepare all emissions data for Typ02G and Base18G simulations. We discuss the sources of all inventory and ancillary data used for simulations. CENRAP worked with emissions inventory contractors, other RPOs, and EPA to collect all of the data that constitute the simulation. Table 2-8 lists all of the contacts for the various U.S. anthropogenic emission inventories we used. For the CENRAP inventories, this table lists the contacts for the contractors who prepared the inventories; for the non-CENRAP inventories it lists the contacts at the RPOs who provided us inventory data. We obtained the emissions inventories for Canada and Mexico from the U.S. EPA Emissions Factors and Inventory Group (EFIG) via the Clearinghouse for Inventories and Emissions Factors (CHIEF) website (<http://www.epa.gov/ttn/chief/index.html>).

Table 2-8. CENRAP anthropogenic emissions inventory contacts.

Source Category	Emissions Data Contact
WRAP	
All	Tom Moore, Western Governors' Association Phone: (970) 491-8837 Email: mooret@cira.colostate.edu
CENRAP	
2002 Consolidated Inventory	Randy Strait, E.H. Pechan & Assoc., Inc. Phone: 919-493-3144 Email: rstrait@pechan.com
NH ₃ Inventory, Prescribed and Agricultural Fires, and On-road mobile emissions	Dana Sullivan, Sonoma Technology, Inc. Phone: 707-665-9900 Email: dana@sonomatech.com
Gulf Off-shore platform and support vessel emissions	Holly Enszt, Minerals Management Service Phone: (504) 736-2536 Email: holli.enszt@mms.gov
VISTAS	
All	Greg Stella, Alpine Geophysics, LLC, Phone: 828-675-9045 Email: gms@alpinegeophysics.com
MANE-VU	
All	Megan Schuster, MARAMA, Baltimore, MD USA Phone: 410-467-0170 Email: mschuster@marama.org
MRPO	
All	Mark Janssen, LADCO, Des Plaines, IL, USA Phone: 847-296-2181 Email: janssen@ladco.org

As mentioned above, the refinement of these inventories involved splitting some of the inventory files into more specific source sectors. As the stationary-area-source emissions sector has traditionally been a catch-all for many types of sources, this is the inventory sector that required the greatest amount of preparation. Upon receiving all stationary-area-source inventories we extracted fugitive dust, road dust, anthropogenic NH₃, and for the non-WRAP U.S. inventories, stage II refueling sources. We retained the dust sources as separate categories that we would further refine with the application of transport factors (see Section 2.8).

We collected the ancillary data used for SMOKE modeling from several sources. SMOKE ancillary modeling data include:

- Temporal and chemical allocation factors by state, county, and source classification code (SCC);
- Spatial surrogates and cross-reference files for allocating county-level emissions to the model grid;
- Hourly gridded meteorology data;
- Stack defaults for elevated point sources;
- MOBILE6 configuration files;

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- A Federal Implementation Standards (FIPS) codes (i.e., country/state/county codes) definition file;
- A Source Category Classification (SCC) codes definition file;
- A pollutant definition file; and
- Biogenic emission factors.

Except for the meteorology data and the MOBILE6 configuration files, we used default data sets provided by EPA as the basis for all of the ancillary data except for temporal profiles used for Electric Generating Units (EGUs). These profiles were developed based on CEM data from 2000 through 2003 (Pechan and CEP, 2005c). CENRAP provided the meteorology data for the simulations at 36-km and 12-km grid resolutions (Johnson, 2007). The inventory contractor who prepared the MOBILE6 inventories provided the MOBILE6 configuration files either directly or via an RPO representative; details about the sources of the MOBILE6 inputs are provided in Section 2.4. We made minor modifications to the chemical allocation, pollutant definition, and country/state/county codes files for new sources, pollutants, or counties contained in the inventories that we had not previously modeled. We made major modifications to the temporal and spatial allocation inputs, as described below.

2.1.7 Temporal Allocation

Temporally allocating annual, daily, or hourly emissions inventories in SMOKE involves combining a temporal cross-reference file and a temporal profiles file.

- Temporal cross-reference files associate monthly, weekly, and diurnal temporal profile codes with specific inventory sources, through a combination of a FIPS (country/state/county) code, an SCC, and sometimes for point sources, facility and unit identification codes.
- Temporal profiles files contain coded monthly, weekly, and diurnal profiles in terms of a percentage of emissions allocated to each temporal unit (e.g., percentage of emissions per month, weekday, or hour).

As a starting point for the temporal allocation data for simulations, we used the files generated by emission inventory contractors (Pechan and CEP, 2005c). Based on guidance from the developers of some of the inventory files, we enhanced the temporal profiles and assignments for some source categories (Pechan, 2005b).

We modified the temporal allocation data for the simulations to improve the representation of temporal emissions patterns for certain source categories. We implemented the adjusted profiles in SMOKE by modifying the temporal cross-reference file for the applicable FIPS and SCC combinations.

Updated temporal profiles for EGUs were made available for MRPO in the MRPO Base K inventory. Since the non-road emissions for IA and MN were monthly emissions developed by MRPO, new temporal profiles were created for all the SCCs in these emissions files for these two states only. The monthly profile was uniform and the weekly and diurnal profiles were kept the same as were modeled for the rest of the country.

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An updated temporal profile, profile 485, based on NOAA 1971-2000 population weighted average heating degree days for home heating area source emissions was obtained from VISTAS. This profile provided state specific updates for home heating emissions and was applied to the full inventory in place of profile 17XX.

Other additions to the Base02G temporal allocation data included updates that made by other RPOs that are applicable to their inventories. These other updates to the temporal allocation files included

- VISTAS continuous emissions monitoring (CEM)-specific profiles for EGUs in the VISTAS states;
- VISTAS agricultural burning profiles;
- Wildfire and prescribed fire profiles developed by VISTAS for the entire U.S.;
- MANE-VU on-road mobile profiles;
- WRAP weekly and diurnal road dust profiles;
- WRAP diurnal wildfire, agricultural fire, and prescribed fire profiles; and
- WRAP on-road mobile weekly and diurnal profiles.

Finally, for all of the monthly and seasonal emissions inventories, we modified the temporal cross-reference files to apply uniform monthly profiles to the sources contained in these inventories. The monthly variability is inherent in monthly and seasonal inventories and does not need to be reapplied through the temporal allocation process in SMOKE. The inventories to which we applied uniform monthly temporal profiles included:

- WRAP, CENRAP, and MRPO non-road mobile sources;
- WRAP on-road mobile sources;
- WRAP road dust; and
- CENRAP anthropogenic ammonia.

2.1.8 Spatial Allocation

SMOKE uses spatial surrogates and SCC cross-reference files to allocate county-level emissions inventories to model grid cells. Geographic information system (GIS)-calculated fractional land use values define the percentage of a grid cell that is covered by standard sets of land use categories. For example, spatial surrogates can define a grid cell as being 50% urban, 10% forest, and 40% agricultural. In addition to land use categories, spatial surrogates can also be defined by demographic or industrial units, such as population or commercial area. Similar to the temporal allocation data, an accompanying spatial cross-reference file associates the spatial surrogates (indexed with a numeric code) to SCCs. Spatial allocation with surrogates is applicable only to area and mobile sources that are provided on a county level basis. Point sources are located in the model grid cells by SMOKE based on the latitude-longitude coordinates of each source. Biogenic emissions are estimated based on 1-km² gridded land use information that is mapped to the model grid using a processing program such as the Multimedia Integrated Modeling System (MIMS) Spatial Allocator (CEP, 2004).

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We used various sources of spatial surrogate information for the U.S., Canada, and Mexico inventories in the simulations. For the U.S. and Canadian sources, we used the EPA unified surrogates available through the EFIG web site (EPA, 2005c). For the 36-km grid, EPA provides these data already formatted for SMOKE on the RPO Unified 36-km domain that we used for the simulations. We modified the spatial surrogates for Canada on the RPO Unified 36-km domain by adopting several surrogate categories that were enhanced by the WRAP. Table 2-9 provides details about the new Canadian spatial surrogates that were developed by the WRAP and used for CENRAP simulations. For modeling Mexico, we used Shapefiles developed for the Big Bend Regional Aerosol and Visibility Observations Study (BRAVO) modeling to create surrogates for Mexico on the RPO Unified 36-km domain (EPA, 2005c).

Table 2-9. New Canadian spatial surrogates.

Attribute	Base02a Code	Shapefile	Reference
Land area	950	can_land93_land	Natural Resources Canada (1993) AVHRR land cover data
Water area	951	can_land93_water	Natural Resources Canada (1993) AVHRR land cover data
Forest land area	952	can_land93_forest	Natural Resources Canada (1993) AVHRR land cover data
Agricultural land area	953	can_land93_agri	Natural Resources Canada (1993) AVHRR land cover data
Urban land area	954	can_land93_urban	Natural Resources Canada (1993) AVHRR land cover data
Rural land area	955	can_land93_rural	Natural Resources Canada (1993) AVHRR land cover data
Airports	956	can_airport	U.S. DOT Bureau of Transportation Statistics (2005) NORTAD 1:1,000,000 scale data
Ports	957	can_port	U.S. DOT Bureau of Transportation Statistics (2005) NORTAD 1:1,000,000 scale data
Roads	958	can_road1m	Natural Resources Canada (2001) National Scale Frameworks data
Rail	959	can_rail1m	Natural Resources Canada (1999) National Scale Frameworks data

2.2 Stationary Point Source Emissions

Stationary-point-source emissions data for SMOKE consist of (1) Inventory Data Analyzer (IDA)-formatted inventory files; (2) ancillary data for allocating the inventories in space, time, and to the Carbon Bond-IV chemistry mechanism used in CMAQ and CAMx; and (3) meteorology data for calculating plume rise from the elevated point sources. This section describes where CENRAP obtained these data, how we modeled them, and the types of QA that we performed to ensure that SMOKE processed the data as expected.

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2.2.1 Data Sources

For the stationary-point-source inventories in Typ02G and Base18G, we used actual 2002 data developed by the RPOs for the U.S., version 2 of the year 2000 Canadian inventory, and the BRAVO 1999 Mexican inventory. The BRAVO inventory was updated with entirely new inventories for the six northern states of Mexico for stationary area, as well as stationary point, on-road mobile, and off-road mobile sources. Emissions for the southern states of Mexico were included for the first time in CENRAP simulations Typ02G and Base18G. These data were provided by ERG, Inc., who completed an updated 1999 emissions inventory for northern Mexico (ERG, 2006b) and delivered these data to the WRAP. The CENRAP stationary-point inventory consisted of annual county-level and tribal data provided in August of 2005 (Pechan and CEP, 2005e). The WRAP (ERG, 2006a) and VISTAS Base G (MACTEC, 2006) stationary-point inventories consisted of an annual data set and monthly CEM data for selected EGUs. The WRAP and VISTAS provided these data directly to CENRAP. We downloaded the MANE-VU stationary-point inventories from the MANE-VU web sites. MRPO base K data was downloaded and processed for SMOKE modeling by Alpine Geophysics under contract from MARAMA. UCR entered into a nondisclosure agreement with Environment Canada to obtain version 2 of the 2000 Canadian point-source inventory. This inventory represented a major improvement over the version of the data that we had used in the preliminary 2002 modeling.

Reductions anticipated from BART controls for electric generating units (EGU) in Oklahoma, Arkansas, Kansas, and Nebraska were included in projections of 2018 emissions. These anticipated reductions were based on actual operating conditions and estimated control efficiencies from utilities.

Newly permitted coal-fired utilities were included in 2018 projections. Conservatively, no IPM projected new units were removed from the simulation with the addition of the permitted facilities.

Due to missing or clearly erroneous stack parameters, several facilities in CENRAP states were relegated to default stack profiles based on SCC in the NEI QA process. Prioritizing for the largest emissions sources, these default parameters were corrected by CENRAP States and updated files were provided to modeling contractors. Final IDA input files Typ02G and Base18G for point sources reflect State corrections.

For coal-fired point and area sources, The EPA Office of Air Quality and Planning Standards (OAQPS) determined that the organic carbon fraction in the speciation profile code "NCOAL" was not representative of most coal combustion occurring in the U.S. This profile has an organic carbon fraction of 20%, which includes an adjustment factor of 1.2 to account for other atoms (like oxygen) attached to the carbon. OAQPS has reverted back to the profile code "22001" for coal combustion, which has an organic carbon fraction of 1.07% (again including the 1.2 factor adjustment). This is the same profile that EPA used for previous rulemaking efforts including the Heavy Duty Diesel Rule and Non-Road Rule, which were proposed (and publicly reviewed) prior to the introduction of the NCOAL profile.

The consensus in OAQPS is that the NCOAL profile has a high organic carbon percentage because it is based on measurements of combustion of lignite coal. With the exception of Texas, lignite is not widely used in the U.S.. Thus, OAQPS staff stopped relying on this profile as a national default profile. A new coal speciation profile developed based on Eastern bituminous

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coal combustion (since much of the coal burned in the U.S. is of this type) is being developed by EPA's Office of Research and Development but was not completed for this study.

The profile recently developed for MRPO by Carnegie Mellon was provided to CENRAP and is representative of combustion of eastern bituminous coal. This profile is a more appropriate profile for most facilities in the U.S. than the default NCOAL profile.

Additionally, the "22001" profile has been flagged as problematic because of the apparent inadvertent switching of the organic carbon and elemental carbon fractions, which are 1.07% and 1.83% respectively. The report discovering the discrepancy in the profile did not offer a clear alternative to correct the problem (MACTEC, 2003).

CENRAP has continued to use the NCOAL factor for facilities burning lignite in North Dakota and Texas. For the remainder of the U.S., the MRPO profile, CMU, was used. The NCOAL factor was modified reducing the organic carbon by half and assigning the remainder to PM_{2.5}. The modification was at the request of Texas and was reflective of the original study for the NCOAL factor conducted in Texas (Chow, 2005). Table 2-10 summarizes the PM_{2.5} speciation profiles for the NCOAL, 2201 and CMU speciation profiles for coal burning sources.

Table 2-10. PM 2.5 speciation profiles for coal-burning sources.

Profile	POC	PEC	PNO3	PSO4	PM2.5
NCOAL	0.1000	0.0100	0.0050	0.1600	0.7250
22001	0.0107	0.0183	0.0000	0.1190	0.8520
CMU	0.0263	0.0315	0.0036	0.0447	0.8938

Final simulations used improved temporal allocation and speciation information relative to the preliminary 2002 modeling; the rest of the ancillary data for modeling stationary point sources stayed the same (Mansell et al., 2005).

2.2.2 Emissions Processing

For Typ02G and Base18G simulations we configured SMOKE to process the annual inventories for the U.S., Canada, and Mexico and process hourly CEM data for the VISTAS. We configured SMOKE to allocate these emissions up to model layer 15 (approximately 2,500 m AGL), which roughly corresponds to the maximum planetary boundary layer (PBL) heights across the entire domain throughout the year. As coarse particulate matter (PMC) is not an inventory pollutant but is required by the air quality models as input species, we used SMOKE to calculate PMC during the processing as (PM₁₀ - PM_{2.5}). With the SMOKE option WKDAY_NORMALIZE set to "No," we treated the annual inventories based on the assumption that they represent average-day data based on a seven-day week, rather than average weekday data. We also assumed that all of the volatile organic compound (VOC) emissions in the inventories are reactive organic gas (ROG), and thus used SMOKE to convert the VOC to total organic gas (TOG) before converting the emissions into CB-IV speciation for the air quality models. To capture the differences in diurnal patterns that are contained in the CEM temporal profiles for VISTAS and CENRAP states (Base02F), we configured SMOKE to generate daily temporal matrices, as opposed to using a Monday-weekday-Saturday-Sunday (MWSS) temporal allocation approach.

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To QA the stationary-point emissions, we used the procedures in the CENRAP emissions modeling QA protocol (Morris and Tonnesen, 2004) and a suite of graphical summaries. We used tabulated summaries of the input data and SMOKE script settings to document the data and configuration of SMOKE for all simulations. These QA graphics are available on the web site at: <http://pah.cert.ucr.edu/aqm/cenrap/emissions.shtml>

2.2.3 Uncertainties and Recommendations

There were issues with the stationary-point emissions that we left unresolved at the completion of the Typ02G and Base18G emissions modeling either because we did not feel they would have a major impact on the modeling results in CENRAP states or because we did not have alternative approaches and they represented the best available information. Canadian emissions for 2000 were found to have a significant number of missing stack parameters. These stacks when modeled with default parameters frequently resulted in lower plume heights. Stack parameters for 2000 were corrected based on cross referencing sources with the 2005 Canadian inventory for the largest emitting points. Stack parameters for many of the sources with lower emissions remain incorrect, but are assumed to have a less significant impact on CENRAP Class I areas. The 2020 projected emissions for Canada were obtained as air quality model-ready files from EPA. EPA has not confirmed that missing stack parameters were corrected for the projected inventory. It is assumed that they were not corrected and default parameters were used instead. Given confidentiality issues that surround Canadian inventories, EPA processed emissions represent the best available data.

2.3 Stationary Area Sources

Stationary-area-source emissions data for SMOKE consist of IDA-formatted inventory files and ancillary data for allocating the inventories in space, time, and to the Carbon Bond-IV chemistry mechanism used in CMAQ and CAMx. This section describes where we obtained these data, how we modeled them, and the types of QA that we performed to ensure that SMOKE processed the data as expected.

2.3.1 Data Sources

For the stationary area source inventories in the Typ02G and Base18G simulations, we used actual 2002 data developed by the RPOs for the U.S., version 2 of the year 2000 Canadian inventory, and the updated Mexican inventory, <http://www.epa.gov/ttn/chief/net/mexico.html>. The BRAVO inventory was updated with entirely new inventories for the six northern states of Mexico for stationary area, as well as stationary point, on-road mobile, and off-road mobile sources. Emissions for the southern states of Mexico were included for the first time in CENRAP simulations Typ02G and Base18G. The CENRAP stationary-area inventory consisted of annual county-level and tribal data provided by in August of 2005 (Pechan and CEP, 2005e). The WRAP (ERG, 2006a) and VISTAS Base G (MACTEC, 2006) stationary-area inventories consisted of an annual data set. We downloaded the MANE-VU stationary-area inventories from the MANE-VU web sites. MRPO base K data was downloaded and processed for SMOKE modeling by Alpine Geophysics under contract from MARAMA.

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To prepare the stationary-area inventories for modeling, we made several modifications to the files by removing selected sources either to model them as separate source categories or to omit them from simulations completely. Using guidance provided by EPA (EPA, 2004b), we extracted fugitive and road dust sources from all stationary-area inventories for adjustment by transport factors and modeling as separate source categories (see Section 2.8). We also extracted and discarded the stage II refueling sources (Table 2-11) from the U.S. inventories; we modeled these sources with MOBILE6 as part of the on-road mobile-source emissions. We left the stage II refueling emissions in the WRAP stationary-area inventory because the on-road mobile inventory that we received for this region did not contain these emissions.

Table 2-11. Refueling SCCs removed from the non-WRAP U.S. stationary-area inventory.

SCC	Description
2501060100	Storage and Transport Petroleum and Petroleum Product Storage Gasoline Service Stations Stage 2: Total
2501060101	Storage and Transport Petroleum and Petroleum Product Storage Gasoline Service Stations Stage 2: Displacement Loss/Uncontrolled
2501060102	Storage and Transport Petroleum and Petroleum Product Storage Gasoline Service Stations Stage 2: Displacement Loss/Controlled
2501060103	Storage and Transport Petroleum and Petroleum Product Storage Gasoline Service Stations Stage 2: Spillage
2501070100	Storage and Transport Petroleum and Petroleum Product Storage Diesel Service Stations Stage 2: Total
2501070101	Storage and Transport Petroleum and Petroleum Product Storage Diesel Service Stations Stage 2: Displacement Loss/Uncontrolled
2501070102	Storage and Transport Petroleum and Petroleum Product Storage Diesel Service Stations Stage 2: Displacement Loss/Controlled
2501070103	Storage and Transport Petroleum and Petroleum Product Storage Diesel Service Stations Stage 2: Spillage

Other steps that we took to prepare the stationary-area inventories included confirming that there is no overlap between the anthropogenic NH₃ inventory (Section 2.9) and stationary area sources, and moving area-source fires in each regional inventory to separate files. In addition to these inventory modifications we made a few changes to the ancillary data files for simulation Typ02G, as described next.

Simulation Typ02G used improved temporal and spatial allocation information relative to the preliminary 2002 modeling; the rest of the ancillary data for modeling stationary area sources stayed the same as in the preliminary 2002 modeling (Mansell et al., 2005). We adopted enhanced spatial allocation data with additional area-based surrogates for Canada (Table 2-9), and added surrogates for a missing county in Colorado (Broomfield) from WRAP modeling and QA work. The WRAP had noticed when looking at the Canadian data for the preliminary 2002 modeling that forest fire emissions from the Canadian area-source inventory, which are relatively large sources of CO, NO_x, and PM_{2.5}, were being allocated to a surrogate for logging activities. They found similar discrepancies for other area and non-road SCCs in Canada. To improve the representation of the Canadian emissions, we adopted several land-area-based surrogates developed by the WRAP, such as forested land area, urban land area, and rural land area, and made the accompanying additions to the spatial cross-reference file to associate inventory SCCs with these surrogates. We also added spatial surrogates for Broomfield County, CO; this county was included in the inventory but was not included in the base EPA surrogates (this county was recently created from portions of other counties).

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Improvements to the temporal allocation data for simulation Typ02G included the addition of several FIPS-specific profiles provided by VISTAS and CENRAP contractors (Pechan 2005b). These temporal profiles listed in Table 2-12 targeted mainly fire and agricultural NH₃ sources, such as open burning and livestock operations, respectively.

Table 2-12. New Temporal Profile Assignments for CENRAP Area Source SCCs.

SCC	Description	Month	Week	Diurnal	Recommendation Based on Profile Data for SCC	Description of Similar SCC used to Recommend Profiles
2310001000	Industrial Processes; Oil and Gas Production: SIC 13;All Processes : On-shore; Total: All Processes	262	7	26	2310000000	Industrial Processes;Oil and Gas Production: SIC 13;All Processes;Total: All Processes
2310002000	Industrial Processes;Oil and Gas Production: SIC 13;All Processes : Off-shore;Total: All Processes	262	7	26	2310000000	Industrial Processes;Oil and Gas Production: SIC 13;All Processes;Total: All Processes
2461870999	Solvent Utilization;Miscellaneous Non-industrial: Commercial;Pesticide Application: Non-Agricultural;Not Elsewhere Classified	258	7	26	2461800000	Solvent Utilization;Miscellaneous Non-industrial: Commercial;Pesticide Application: All Processes;Total: All Solvent Types
2805009200	Miscellaneous Area Sources;Agriculture Production - Livestock;Poultry production - broilers;Manure handling and storage	1500	7	26	2805009300	Miscellaneous Area Sources;Agriculture Production - Livestock;Poultry production - broilers;Land application of manure
2805021100	Miscellaneous Area Sources;Agriculture Production - Livestock;Dairy cattle - scrape dairy;Confinement	1500	7	26	2805021300	Miscellaneous Area Sources;Agriculture Production - Livestock;Dairy cattle - scrape dairy;Land application of manure
2805021200	Miscellaneous Area Sources;Agriculture Production - Livestock;Dairy cattle - scrape dairy;Manure handling and storage	1500	7	26	2805021300	Miscellaneous Area Sources;Agriculture Production - Livestock;Dairy cattle - scrape dairy;Land application of manure
2805023100	Miscellaneous Area Sources;Agriculture Production - Livestock;Dairy cattle - drylot/pasture dairy;Confinement	1500	7	26	2805023300	Miscellaneous Area Sources;Agriculture Production - Livestock;Dairy cattle - drylot/pasture dairy;Land application of manure
2805023200	Miscellaneous Area Sources;Agriculture Production - Livestock;Dairy cattle - drylot/pasture dairy;Manure handling and storage	1500	7	26	2805023300	Miscellaneous Area Sources;Agriculture Production - Livestock;Dairy cattle - drylot/pasture dairy;Land application of manure
2810020000	Miscellaneous Area Sources;Other Combustion;Prescribed Burning of Rangeland;Total	3	11	13	2810015000	Miscellaneous Area Sources;Other Combustion;Prescribed Burning for Forest Management;Total

2.3.2 Emissions Processing

For simulations Typ02G and Base18G we configured SMOKE to process the annual stationary-area-source inventories for the U.S., Canada, and Mexico. As PMC is not an inventory pollutant but is required by the air quality models as input species, we used SMOKE to calculate PMC during the processing as (PM₁₀ - PM_{2.5}). With the SMOKE option WKDAY_NORMALIZE set to “Yes,” we treated the annual stationary-area inventories based on the assumption that they represent average weekday data, causing SMOKE to renormalize the data to a seven-day estimate before applying any temporal adjustments. We also assumed that all of the VOC emissions in the inventories are ROG and thus used SMOKE to convert the VOC to TOG before converting the emissions into CB-IV speciation for the air quality models. We configured SMOKE to use a MWSS temporal allocation approach, as opposed to a daily temporal approach.

To QA the stationary-area emissions, we used the procedures in the CENRAP modeling QAPP and Modeling Protocol (Morris and Tonnesen, 2004; Morris et al., 2004a) and a suite of graphical summaries. We used tabulated summaries of the input data and SMOKE script settings to document the data and configuration of SMOKE for all simulations. The graphical QA summaries include, for all emissions output species, daily spatial plots summed across all model layers, daily time-series plots, and annual time-series plots. These QA graphics are available on the UCR/CENRAP web site at <http://pah.cert.ucr.edu/aqm/cenrap/emissions.shtml>.

2.3.3 Uncertainties and Recommendations

Most of the issues that we encountered with the stationary area sources related to the removal of certain SCCs from the base inventories for inclusion as other source categories or complete omission from simulations. We spent considerable effort on ensuring that we did not have overlap between the area inventory and the other sectors that explicitly represent sources traditionally contained in the area inventory, such as NH₃ and dust.

Both the Canadian and Mexican inventories presented minor problems that we resolved for simulation Typ02G but that can be addressed more thoroughly in future simulations. The Canadian inventory we used contained data only at the province level, essentially equivalent to a statewide rather than county-level inventory. A higher resolution inventory would have allowed us to use higher-resolution and more accurate spatial allocation data. Future modeling that uses Canadian data should move to the newly released municipality-level year 2000 inventories for Canada.

There was a discrepancy between the state and county coding in the Mexican inventory and the SMOKE file that defines acceptable FIPS codes. Differences in the ordering of the Mexican state names between these two data sets led to some of the Mexican inventory sources being mislabeled in the SMOKE QA reports. The state codes in the inventory and spatial surrogate files for two Mexican states were changed to be consistent with the SMOKE country/state/county codes file.

2.4 On-Road Mobile Sources

On-road mobile-source emissions data for SMOKE consist of IDA-formatted emissions and vehicle activity inventory files, and ancillary data for allocating the inventories in space, time, and to the Carbon Bond-IV chemistry mechanism used in CMAQ and CAMx. This section describes where we obtained these data, how we modeled them, and the types of QA that we performed to ensure that SMOKE processed the data as expected.

2.4.1 Data Sources

The SMOKE processing for CENRAP included two approaches for processing on-road mobile sources depending on the source of the data provided. The first approach was to compute mobile emissions values prior to providing them to SMOKE; we call this the pre-computed emissions approach. The second approach was to provide SMOKE with VMT data, meteorology data, and MOBILE6 inputs, and let the SMOKE/MOBILE6 module compute the mobile emissions based on these data; we call this the VMT approach. These approaches are not mutually exclusive for a single SMOKE run; therefore, we performed single SMOKE runs in which both approaches were used as follows:

- Annual VMT for computing CO, NO_x, VOC, SO₂, NH₃ and PM using MOBILE6 for all CENRAP States.
- Pre-computed, seasonal MOBILE6-based emissions of all pollutants for the 13 WRAP states that included pre-specified PM_{2.5} data.
- Annual VMT for computing CO, NO_x, VOC, SO₂, NH₃ and PM using MOBILE6 for the rest of the United States (VISTAS, MRPO and MANE-VU).
- Pre-computed, annual 1999 emissions of all pollutants for Mexico.
- Pre-computed, annual 2000 emissions of all pollutants for Canada.

For the CENRAP states, STI provided VMT data and MOBILE6 input files for all counties in the CENRAP region (Reid et al., 2004a). MOBILE6 input files were provided only for the months of January and July for 2002. MOBILE6 input files for the remaining months of 2002 had to be generated. These data were then processed within SMOKE. Using one set of MOBILE6 input files for each county in the CENRAP states resulted in compute memory requirements that were too large to process all CENRAP states together. Therefore the on-road mobile processing for the CENRAP states was split into two groups for SMOKE processing. The resulting gridded emissions data files were then merged together to obtain an on-road mobile source emissions file for the entire CENRAP region.

For the WRAP states we used actual 2002 data split into California and non-California seasonal inventories that were provided by the WRAP (Pollack et al., 2006). In addition to the standard criteria pollutants, these files contained pre-specified PM_{2.5} emissions. For the rest of the U.S. we used annual county-level activity and speed inventories with monthly, county-level MOBILE6 inputs, and hourly meteorology to estimate the hourly emissions with the SMOKE/MOBILE6 module. For the non-U.S. inventories, we used version 2 of the year 2000 Canadian inventory and the updated 1999 Mexican inventory pre-computed mobile source emissions.

2.4.2 Emissions Processing

For the Typ02G emissions modeling we configured SMOKE to process the annual on-road mobile emissions inventory data for the WRAP, Canada, and Mexico as pre-computed inventories. For the non-WRAP states, we used the SMOKE/MOBILE6 integration to process the annual activity inventories and monthly, county-based roadway information. The WRAP inventories contained pre-computed speciated PM emissions (Pollack et al, 2006) so the SMOKE PM speciation module was not used. The WRAP on-road mobile inventories were developed to represent seven-day (weekly) average emissions (as compared to the area source inventory, which represented average weekday emissions). As actual weekly average emissions, we configured SMOKE to process the WRAP on-road mobile source emissions by setting WKDAY_NORMALIZE to “No” in which case the emissions are adjusted to represent weekday and Saturday and Sunday emissions (as in contrast to the area sources where the emissions are just adjusted for Saturday and Sunday). We also assumed that all of the VOC emissions in the inventories are ROG and used SMOKE to convert the VOC to TOG before converting the emissions into CB-IV speciation for the air quality models. We configured SMOKE to create day-of-week specific rather than MWSS, temporal profiles because the WRAP on-road mobile temporal profiles contain weekly profiles that vary across the weekdays.

As noted previously, the large number of county roadway inputs for MOBILE6 processed for the non-WRAP portion of the U.S. required us to split the states mobile-source processing into three subsets because of computer memory limitations. Separate MOBILE6 input files were used for each separate county for CENRAP states, where as one MOBILE6 input file was used for several counties outside of the CENRAP region. The three subsets consisted of two sets of SMOKE/MOBILE6 simulations for the CENRAP and a simulation that computed on-road mobile emissions for the MRPO, VISTAS, and MANE-VU states. We configured MOBILE6 to use weekly temperature averaging for computing these emissions within SMOKE.

To QA the on-road mobile emissions, we used the CENRAP emissions modeling QA protocol (Morris and Tonnesen, 2004; Morris et al., 2004a) and a suite of graphical summaries. We used tabulated summaries of the input data and SMOKE script settings to document the data and configuration of SMOKE for simulations Typ02G and Base18G. The graphical QA summaries include, for all emissions output species, daily spatial plots, daily time-series plots, and annual time-series plots. These graphics are available at http://pah.cert.ucr.edu/aqm/cenrap/qa_base02b36.shtml#mb

2.4.3 Uncertainties and Recommendations

We approached the on-road mobile emissions preparation for simulation Typ02G from three different directions, which were based on the form of the input inventories and ancillary emissions data for different regions of the modeling domain:

- The WRAP region used emissions estimates pre-computed with EMFAC for California and MOBILE6 for the rest of WRAP states and processed like area sources with SMOKE adjusted from weekly to day-of-week emissions.
- The CENRAP, VISTAS, MRPO, and MANE-VU states used county-level activity data to compute emissions with the SMOKE/MOBILE6 module.

- The non-U.S. parts of the domain also had pre-computer on-road mobile source emissions so used an area-source approach for processing with SMOKE.

Different approaches for modeling a single emissions sector adds complexity and additional sources of error and inconsistencies to the modeling because of the different assumptions that went into the preparation of the input data. For example, refueling emissions from the on-road mobile sector are represented in the WRAP area-source sector but are computed with MOBILE6 for the rest of the U.S. Not using MOBILE6-based emissions for the non-U.S. portion of the domain neglects the effects of the actual 2002 meteorology on these emissions. Applying MOBILE6 outside of the U.S. is currently not possible because MOBILE6 is instrumented only for calculating emissions for the U.S. automotive fleet. The result of using MOBILE6 to calculate U.S. emissions and not using it to calculate the non-U.S. on-road mobile emissions estimates is that the non-U.S. emissions are not specific to this modeling year and the 2002 meteorological conditions, whereas the U.S. emissions are 2002-specific.

While we used the best available information to compute the on-road mobile emissions for the various portions of the modeling domain, inconsistent approaches for representing these emissions may lead to unnatural emissions gradients along political boundaries. We recommend for future work a unified approach for at least the U.S. inventories, where either we use MOBILE6 in SMOKE for the entire domain (or alternative emissions model such as CONCEPT), or we calculate the emissions with MOBILE6 outside of SMOKE and then use the resulting county-based emissions inventories.

2.5 Non-Road Mobile Sources

Non-road mobile source emissions data for SMOKE consist of annual, seasonal, and monthly IDA-formatted emission inventory files and ancillary data for allocating the inventories in space, time, and to the Carbon Bond-IV chemistry mechanism used in CMAQ and CAMx. This section describes where we obtained these data, how we modeled them, and the types of QA that we performed to ensure that SMOKE processed the data as expected.

2.5.1 Data Sources

The non-road mobile-source inventories in the Typ02G and Base18G emissions modeling used actual 2002 data developed by the RPOs for the U.S., version 2 of the year 2000 Canadian inventory and the improved 1999 Mexican inventory. The U.S. inventories consisted of annual, seasonal, and monthly inventories; the non-U.S. inventories were annual data. Pechan provided the CENRAP inventories divided between annual data for aircraft, locomotive, and commercial marine and annual files for all other non-road sources (Pechan and CEP, 2005e). Minnesota substituted the monthly MRPO Base K non-road inventory for the CENRAP inventory in their state. Iowa substituted the monthly estimates for non-road agricultural sources from the MRPO base K inventory for the CENRAP inventory. Texas provided estimates for 2002 non-road emissions in lieu of the CENRAP prepared inventory. WRAP provided non-road inventories divided between California and non-California seasonal inventories, further subdivided into aircraft, locomotives, shipping, and all other non-road mobile sources (Pollack et al., 2006). Note that the California Air Resources Board uses their own OFFROAD model for California non-road emissions, whereas the EPA NONROAD model is used for the rest of the states (with the

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exception of locomotives, aircraft and shipping). With these data WRAP also provided temporal adjustments to apply to the inventories to split them between weekday and weekend emissions. We used these weekday/weekend splits to derive new weekly temporal profiles for the WRAP sources. The MRPO base K monthly non-road inventories were obtained from MRPO in NIF format and were converted to SMOKE format by Wendy Vit of the Missouri DNR. The VISTAS Base G and MANE-VU non-road mobile inventories consisted of annual county-level data (Pechan and CEP, 2005c). We received these inventories directly from the respective RPO inventory representatives. We received the Canadian 2000 inventory version 2 from the U.S. EPA EFIG (EPA, 2005d). For Mexico we used the improved 1999 inventory available at <http://www.epa.gov/ttn/chief/net/mexico.html>.

Along with adding the WRAP weekday/weekend emissions splits to the temporal allocation files, we also created temporal input files that apply a flat, uniform monthly profile to the monthly and seasonal non-road inventories. With the monthly and seasonal variability inherent in these inventories, we avoided applying redundant monthly profiles by splitting the inventories into seasonal/monthly and annual data. We applied the uniform monthly temporal profiles to the seasonal/monthly inventories and non-uniform monthly temporal profiles to the annual inventories. How the non-road emissions inventory data were split into those with monthly/seasonal emission and those with annual emissions is provided in Table 2-13.

Table 2-13. Non-road mobile-source inventory temporal configuration.

Region	Source	Temporal Coverage
WRAP (non-CA)	Non-road mobile	Seasonal
WRAP (CA)	Non-road mobile	Seasonal
WRAP	Aircraft	Seasonal
WRAP	Locomotive	Annual
WRAP	In-port and near-shore shipping	Annual
CENRAP	All non-road	Annual
CENRAP, IA	Non road Ag.	Monthly
VISTAS	All non-road	Annual
MRPO and MN	All non-road	Monthly
MANE-VU	All non-road	Annual
Canada	All non-road	Annual
Mexico	All non-road	Annual

Iowa elected to use the CENRAP-sponsored inventory for all of the non-road categories except for the agricultural equipment categories provided in Table 2-14. For these agricultural equipment categories, Iowa elected to use the Midwest RPO Base K inventory because this inventory provided improvements to the temporal allocation of emissions for the agricultural sector. The Base K inventory includes monthly emissions. The monthly emissions are used in the SMOKE IDA files for modeling.

Table 2-14. Non-road agricultural emissions categories where the MRPO Base K inventory was used instead of the CENRAP inventory in Iowa.

SCC	SCC Description
22600050xx	Off-highway Vehicle Gasoline, 2-Stroke: Agricultural Equipment (2 SCCs);
22650050xx	Off-highway Vehicle Gasoline, 4-Stroke: Agricultural Equipment (11 SCCs);
22670050xx	LPG : Agricultural Equipment (3 SCCs);
22680050xx	CNG : Agricultural Equipment (3 SCCs); and
22700050xx	Off-highway Vehicle Diesel : Agricultural Equipment (11 SCCs).

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Texas provided annual and daily emissions for CO, CO₂, NO_x, VOC, SO₂, PM10-FIL, and PM25-FIL for several oil and gas field equipment non-road categories (Table 2-15). Texas provided authorization to change the pollutant codes from PM10-FIL to PM10-PRI and PM25-FIL to PM25-PRI.

Table 2-15. Non-road oil and gas development equipment categories that Texas provided emissions to be used instead of the CENRAP inventory.

SCC	SCC Description
2265010010	Off-highway Vehicle Gasoline, 4-Stroke : Industrial Equipment: Other Oil Field Equipment;
2268010010	CNG : Industrial Equipment : Other Oil Field Equipment; and
2270010010	Off-highway Vehicle Diesel : Industrial Equipment : Other Oil Field Equipment

Lancaster County Nebraska provided its own non-road inventory for SCC 2260000000 (Off-highway Vehicle Gasoline, 2-Stroke : 2-Stroke Gasoline except Rail and Marine: All). The CENRAP-sponsored inventories for SCCs starting with 226 in Lancaster County were removed to correct double-counting of emissions. This adjustment was made by Pechan for Base02b modeling.

2.5.2 Emissions Processing

We configured SMOKE to process all of the non-road mobile emissions inventory data as area-like inventories using spatial surrogates to grid the county-level emissions. As the WRAP inventories contained pre-computed PM emissions, we did not have to use SMOKE to compute coarse mass PM (PMC). The WRAP non-road mobile inventories represented seven-day average emissions (different from the area inventory, which represented weekday average emissions). As actual weekly average emissions, we configured SMOKE to process them by setting WKDAY_NORMALIZE to “No.” For the rest of the non-road mobile inventories we processed the data as weekday average data by setting WKDAY_NORMALIZE to “Yes.” We also assumed that all of the VOC emissions in the inventories are ROG and used SMOKE to convert the VOC to TOG before converting the emissions into CB-IV speciation for the air quality models. We configured SMOKE to create MWSS temporal intermediates rather than daily temporal files because the non-road mobile sources do not use weekly temporal profiles that vary across the weekdays, but do have very different emissions on weekdays versus weekend days.

We divided the non-road mobile emissions modeling based on whether the data were annual or seasonal/monthly inventories. This split facilitated the application of uniform monthly temporal profiles to the seasonal/monthly inventories. After processing the non-road emissions as two separate categories, non-road yearly and non-road monthly, we combined them with the rest of the emissions sectors to create model-ready emissions for CMAQ and CAMx.

To QA the non-road mobile emissions we used the procedures in the CENRAP emissions modeling QAPP (Morris and Tonnesen, 2004) and Modeling Protocol (Morris et al., 2004a) and a suite of graphical summaries. We used tabulated summaries of the input data and SMOKE script settings to document the data and configuration of SMOKE for simulations. The graphical QA summaries include, for all emissions output species, daily spatial plots, daily time-series plots, and annual time-series plots. These QA graphics are available at

http://pah.cert.ucr.edu/aqm/cenrap/qa_base02f36.shtml#nr

2.5.3 Uncertainties and Recommendations

We prepared non-road mobile emissions using a combination of inventories having different temporal resolutions and various forms of ancillary data. These different combinations of information may lead to inconsistencies in how these emissions are represented across the modeling domain. In addition, the Canadian inventories contain only province-level information and thus have low-resolution spatial and temporal profiles applied to them. The Mexican non-road emissions are deficient in the number of different SCCs contained in the inventory and the availability of spatial surrogates that are applicable to non-road mobile sources. Improvements to the temporal profiles and spatial surrogates could provide a more consistent approach to representing the non-road emissions across the entire modeling domain.

2.6 Biogenic Sources

Biogenic emissions data for SMOKE consist of input files to the BEIS3 model (EPA, 2004a). BEIS3 is a system integrated into SMOKE for deriving emissions estimates of biogenic gas-phase pollutants from land use information, emissions factors for different plant species, and hourly, gridded meteorology data. The results of BEIS3 modeling are hourly, gridded emissions fluxes formatted for input to CMAQ or CAMx. This section describes the sources of the BEIS3 input data that we used for the Typ02G and Base18G emissions, how we modeled these data and the types of QA that were performed to ensure that SMOKE processed the data as expected.

2.6.1 Data Sources

The BELD3 land use data and biogenic emissions factors that were developed during the WRAP preliminary 2002 modeling were used for the CENRAP biogenic emissions modeling (Tonnesen et al., 2005). These data included BELD3 1-km resolution land use estimates and version 0.98 of the BELD emissions factors. Since the WRAP and CENRAP use the same 36 km Inter-RPO continental U.S. modeling domain, CENRAP was able to leverage of the WRAP work performed previously.

2.6.2 Emissions Processing

We used BEIS3.12 integrated in SMOKE to prepare emissions for the simulations. Most of the preparation for the biogenic emissions processing was completed during the preliminary 2002 modeling (Morris et al., 2005). As the modeling domains did not change from the preliminary 2002 to the final modeling, we re-used the gridded land use data and vegetation emissions factors that we prepared for the preliminary simulations.

To QA the biogenic emissions, we used the CENRAP emissions modeling QAPP (Morris and Tonnesen, 2004) and Modeling Protocol (Morris et al., 2004a) and a suite of graphical summaries. We used tabulated summaries of the input data and SMOKE script settings to document the data and configuration of SMOKE for simulation Base02b. The graphical QA summaries include, for all emissions output species, daily spatial plots, daily time-series plots, and annual time-series plots. These QA graphics are available at http://pah.cert.ucr.edu/aqm/cenrap/qa_base02b36.shtml#b3

2.6.3 Uncertainties and Recommendations

The use of newer versions of BEIS (BEIS3.13) and the new MEGAN biogenic emissions models should be considered in future modeling.

2.7 Fire Emissions

Fire emissions data for SMOKE have traditionally been represented as county-level area-source inventories that were placed in only the first vertical model layer. We advanced the representation of fire emissions for air quality modeling by preparing portions of the inventory data as point sources with specific latitude-longitude coordinates for each fire centroid and pre-computed plume rise parameters that were derived from individual fire characteristics. These new inventories were based on the fire data products prepared by a CENRAP emission contractor (Reid et al., 2004b) and modified by the project team to be properly modeled as point sources. These data consist of annual, daily, and hourly IDA-formatted emissions inventory files and ancillary data for allocating the inventories in space, time, and to the Carbon Bond-IV chemistry mechanism used in CMAQ and CAMx. This section describes where we obtained these data, how we modeled them, and the types of QA performed to ensure that SMOKE processed the fire emissions data as expected.

2.7.1 Data Sources

The fire inventories in the Typ02G emissions inventory were held constant through Base18G. We used actual 2002 fire data developed by the RPOs for the U.S., version 2 of the year 2000 Canadian inventory fire data, and actual 2002 fire data for Ontario, Canada. The inventories used consisted of both area and point source data for the U.S., Canada, and Mexico. Sonoma Technology, Inc. provided the fire emissions for the CENRAP states (Reid et al., 2004b). Air Sciences provided us with the WRAP inventories divided among six different fire categories: wildfires, agricultural fires, wildland fire use, natural prescribed, anthropogenic prescribed, and non-Federal rangeland fires (Air Sciences, 2007a). These inventories consisted of annual, daily, and hourly IDA-formatted files with information on daily emissions totals and hourly plume characteristics for each fire. We received similar fire emission inventories for the other RPOS (Air Sciences, 2007b). We modeled these sources with the rest of the stationary-area-source sector.

CENRAP received data for 54 fires that occurred in Ontario during the year 2002. Information on the data code abbreviations, data definitions, and data units used in the raw data files was obtained from Mr. Rob Luik (Data Management Specialist) at the Ontario Ministry of Natural Resources (Rob.Luik@MNR.gov.on.ca). Emissions for each fire were estimated using the Emission Production Model (EPM)/CONSUME within the BlueSky framework. A fire identification code is needed to track individual fires throughout the processing. The unique fire identification code was created for each fire by concatenating the FIRE_NUMBER and CUR_DIST fields of the original data. The fire identification code also contains the FIPS code of the fire; this information is not used by BlueSky but is needed by BlueSky2Inv, the utility program that converts the BlueSky output to the SMOKE inventory format. The FIPS code 135000 was used for all fires with longitudes east of -90° , and FIPS code 135059 was used for

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fires west of -90° . These FIPS codes were used to ensure that the fires would be assigned the correct time zones in later SMOKE processing. Some of the dates provided in the original data included hourly information. In all cases, the hourly information was not used leaving all data at a daily resolution.

2.7.2 Emissions Processing

SMOKE is instrumented to distribute point-source-formatted fire inventories to the vertical model layers either by using a pre-computed plume rise approach or by computing the plume rise dynamically using actual 2002 meteorology. We applied both approaches for modeling point-source fire emissions in simulation Typ02G. For the pre-computed plume rise approach, SMOKE reads an annual inventory file with information on fire locations, a daily inventory file with daily emission totals for each fire, and an hourly inventory file with hourly plume bottom, plume top, and layer 1 fractions for each fire. SMOKE uses this information to locate the fires on the horizontal model grid and to distribute the plume of each fire vertically to the model layers. Because some of these fires have plumes that reach the model top, we set the number of emissions layers for processing these inventories to the full 19 layers of the meteorology. We applied this approach to the point-source fires for the WRAP, CENRAP and VISTAS regions. The alternative plume rise approach uses information on fuel loading and the heat flux of the fires to distribute the fires vertically to the model layers. The data are provided to SMOKE in the form of an annual inventory with information on fire locations and a daily inventory with daily emission totals for each fire, daily heat flux, and daily fuel loading. We applied this approach to the point-source fires for Ontario, Canada.

All of the point-source fires used diurnal temporal profiles and speciation profiles for VOC and $PM_{2.5}$ developed by Air Sciences (2007a) during the preliminary 2002 modeling (Morris et al., 2005).

We modeled the area-source fires for U.S. and Canada as standard stationary area sources. We applied monthly temporal profiles provided by RPOs, flat weekly temporal profiles, and the diurnal profiles developed by Air Sciences for WRAP fires (Air Sciences, 2007a), and for the rest of the RPOs we used diurnal profiles that were provided by them (Air Sciences, 2007b). We used the forestland area surrogate to distribute these emissions from the county or province level in the inventories to the model grid cells.

To QA the fire emissions, we used the procedure in the CENRAP emissions modeling QA protocol (Environ, 2004) and a suite of graphical summaries. We used tabulated summaries of the input data and SMOKE script settings to document the data and configuration of SMOKE for simulation Typ02G. The graphical QA summaries include, for all emissions output species, daily spatial plots, daily time-series plots, annual time-series plots, and vertical profiles. These QA graphics are available at: http://pah.cert.ucr.edu/aqm/cenrap/qa_typ02g36.shtml.

2.7.3 Uncertainties and Recommendations

We used forestland spatial surrogates to distribute these county level (province level for Canada) data to the model grid. Using spatial surrogates to locate fires is a crude approach that results in the artificial smearing of the emissions over too large an area. This issue can be remedied by

moving to a point-source approach for representing these fires, similar to the approach used by Air Sciences for preparing the WRAP fire inventories.

2.8 Dust Emissions

Dust emissions data for SMOKE have traditionally taken the form of county-level stationary-area-source inventories. As these emissions are correlated to meteorology, land use, and vegetative cover, we made several changes to how dust emissions are simulated by SMOKE to take these parameters into consideration. This section describes where we obtained data for windblown, fugitive, and road dust sources, how we modeled them, and the types of QA performed to ensure that SMOKE processed the data as expected.

2.8.1 Data Sources

For the fugitive dust and road dust inventories in the Typ02G emission scenario, we used actual 2002 data developed by the RPOs for the U.S., version 2 of the year 2000 Canadian inventory, and the BRAVO 1999 Mexican inventory. We extracted the fugitive dust inventories from the stationary-area inventories for each of the RPOs, Mexico, and Canada. Before modeling these data we further divided them into construction/mining sources and agricultural sources. We defined the fugitive dust sources in the Base02f modeling based on guidance provided by EPA (2004b). WRAP provide road dust emission inventories (Pollack et al., 2006). For the rest of the RPOs and Canada, we extracted the road dust SCCs from the stationary-area-source inventories. The BRAVO 1999 Mexico inventory did not contain any road dust SCCs. Table 2-16 lists the SCCs for the various fugitive and road dust sources that we modeled in the Base02f and Typ02G inventories. We applied near-source capture transport factors that are based on county-level vegetative cover to the fugitive and road dust inventories to prepare them for input to the air quality models.

For windblown dust, we used gridded emissions prepared outside of SMOKE using a land use and meteorology-based model developed under funding from the WRAP by ENVIRON and UC-Riverside (Mansell, 2005; Mansell et al., 2005).

Table 2-16. Fugitive and road dust SCCs.

Dust Category	SCCs
Fugitive dust (construction and mining)	2275085000, 2311000000, 2311010000, 2311010070, 2311020000, 2311030000, 2325000000, 2305070000, 2530000020, 2530000100, 2530000120
Fugitive dust (agricultural)	2801000003, 2801000005, 2801000008, 2805001000
Road dust	2294000000, 2296000000

2.8.2 Emissions Processing

We modeled the fugitive and road dust inventories through SMOKE using an area-source approach. We modeled these data on the assumption that they represented weekday, rather than seven-day week, emissions and thus used the SMOKE setting WKDAY_NORMALIZE to convert the data to a seven-day average. We configured SMOKE to compute PMC during the processing as (PM₁₀ - PM_{2.5}). Usually the records with dust do not include any other pollutants such as VOC, and NO_x. For the few records that did include pollutants other than the PM we

split the records where the PMs processed with dust and the non PMs processed with the area. We configured SMOKE to create MWSS temporal intermediates rather than daily temporal files because the dust sources do not use weekly temporal profiles that vary across the weekdays.

As noted above, we used SMOKE to apply near-source transport factors to the raw fugitive and road dust inventories to prepare them for input to the air quality models. We used U.S. transport factors from work done by Pace (2005) and a 2001 land use/land cover database to develop a SMOKE input file of county and SCC-based transport factors for the U.S., Canada, and Mexico. We applied these factors to create a new set of inventories adjusted for these transport factors for all regions except VISTAS; the VISTAS dust sources that we received already had the transport factors applied to them.

We calculated the windblown dust emissions outside of SMOKE using an internally developed, process-based model. By “process-based” we refer to an emissions model that integrates information about the processes that lead to the emissions of interest, in this case windblown dust. The process-based windblown dust model developed by the WRAP considers wind speeds, precipitation history, and soil types to derive gridded dust fluxes resulting from wind disturbances for the modeling domain. More information on this model, its modes of operation, and the configuration used for simulation Base02a are available in Mansell et al. (2005).

To QA the fire emissions, we used the procedures in the CENRAP emissions modeling QAPP (Morris and Tonnesen, 2004) and Modeling Protocol (Morris et al., 2004a) and a suite of graphical summaries. We used tabulated summaries of the input data and SMOKE script settings to document the data and configuration of SMOKE for Base02f emissions. The graphical QA summaries include, for all emissions output species, daily spatial plots, daily time-series plots, and annual time-series plots. These QA graphics are available at http://pah.cert.ucr.edu/aqm/cenrap/qa_base02f36.shtml#fd for fugitive dust, http://pah.cert.ucr.edu/aqm/cenrap/qa_base02f36.shtml#rd for road dust, and http://pah.cert.ucr.edu/aqm/cenrap/qa_base02b36.shtml#wbd for windblown dust.

2.8.3 Uncertainties and Recommendations

There are several improvements that should be made to the dust emissions modeling in future simulations. We will expand the list of fugitive dust SCCs that we extract from the stationary-area-source inventories for application of transport factors. This expanded list is based on recent work by EPA (2004b). We will also explore improvements to the assumptions that we used for generating emissions with the WRAP windblown dust model. Areas of improvement in the windblown dust model include refinements to the land use data and soil characteristics, additional information about agricultural activities in the WRAP and CENRAP regions, detailed model evaluation on targeted windblown dust case studies, and the application of snow-cover and vegetative transport factors to these emissions (Mansell et al., 2005).

2.9 Ammonia Emissions

Ammonia (NH₃) emissions from agricultural activities are a major source of ammonia and are dependent on many different environmental parameters, such as meteorology, crop and soil types, and land use. CENRAP developed NH₃ emissions for the CENRAP states (Pechan and CEP, 2005e). Ammonia emissions were estimated for 13 source categories using the Carnegie

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Mellon University (CMU) model and supplemental technical work; 80% of technical work was dedicated to improving emissions estimates for two source categories—livestock production and fertilizer use. For these two categories, as well as biogenic sources, improvements were made to the activity data and/or emission factors used by the CMU model. For four other source categories (industrial point sources, landfills, ammonia refrigeration, and non-road mobile sources), emissions estimates were prepared independently of the CMU model, and for the remaining six source categories (publicly owned treatment works, wildfires, domestic animals, wild animals, human respiration, and on-road mobile sources), emissions estimates were derived by running the CMU model with no alterations.

CENRAP NH₃ model emissions estimates were combined with data provided by the other RPOs to represent agricultural NH₃ emissions in simulations Typ02G and Base18G.

2.9.1 Data Sources

The WRAP provided NH₃ emissions using the WRAP NH₃ model (Mansell et al, 2005) that generated emissions for the following sectors: domestic sources, wild animals, fertilizers, soils, and livestock. MWRPO provided monthly IDA-formatted inventories reflective of base K to CENRAP that they produced from process-based models of their own, along with temporal profiles and spatial cross-reference information for these sources. Iowa elected to use the MWRPO estimates of NH₃ emissions for fertilizer application, livestock, and wastewater treatment or SCC 28017XXXXX, 28050XXXXX, and 2630020000 respectively. Minnesota reviewed the MWRPO inventory and chose to move forward with the CENRAP developed data set. The rest of the U.S., Canada, and Mexico had agricultural NH₃ emissions contained within their annual stationary-area-source inventories.

2.9.2 Emissions Processing

The WRAP NH₃ emissions were processed outside of SMOKE using the WRAP NH₃ model and provided to CENRAP as gridded, hourly emissions in network common data form (NetCDF) files. CENRAP and MWRPO provided monthly IDA-formatted, county-level NH₃ inventories that were developed separately with process-based models. We modeled these emissions like area sources with SMOKE, applying the temporal profiles and the spatial cross-referencing developed for CENRAP that we received from the MWRPO. The agricultural NH₃ emissions for the rest of the RPOs, Canada, and Mexico are contained within their stationary-area inventories. We applied the SMOKE default temporal profiles and spatial surrogates to all non-process-based NH₃ emissions.

To QA the NH₃ emissions, we used the procedures in the CENRAP modeling QAPP (Morris and Tonnesen, 2004) and Modeling Protocol (Morris et al., 2004a) and a suite of graphical summaries. We used tabulated summaries of the input data and SMOKE script settings to document the data and configuration of SMOKE for simulations Typ02G and Base18G. The graphical QA summaries include, for all emissions output species, daily spatial plots, daily time-series plots, and annual time-series plots. These QA graphics are available at <http://pah.cert.ucr.edu/aqm/cenrap/index.shtml>

2.9.3 Uncertainties and Recommendations

Like the other emissions categories that have traditionally been represented as stationary area sources, the agricultural NH₃ emissions sector is affected by interregional inconsistencies in the way these emissions are represented.

During the QA of the Base02a emissions, the WRAP discovered a problem with their soil NH₃ estimates. The emission factor for soil NH₃ that were used in developing these data produced too high an emission estimate from this sector. For simulations Base02B through Typ02G, we therefore removed the soil NH₃ sector completely from the WRAP domain. In future simulations we will include these emissions with a revised emission factor for NH₃ emissions from soils.

2.10 Oil and Gas Emissions

Emissions from oil and gas development activities have been poorly characterized in the past. Simulations These emissions have been sporadically reported by some states in their stationary-area-source inventories, but for the most part were missing from our preliminary modeling. In the Typ02G and Base18G simulations, significant effort was made to better represent oil and gas production emissions explicitly as both area and point sources.

2.10.1 Data Sources

Emissions from oil and gas production activities for the CENRAP states were included with the other CENRAP state emission source categories (Pechan and CEP, 2005e). We received oil and gas production emissions inventories for the WRAP states and for tribal lands in the WRAP region as stationary-area-source and stationary-point-source IDA-formatted inventories. ERG, Inc. provided the point-source inventories with the rest of the stationary-point data (ERG, 2006a). ENVIRON provided the area-source oil and gas inventories for non-CA WRAP states and for tribal lands in the WRAP region, along with spatial surrogates for allocating these data to the model grid (Russell and Pollack. 2005). Oil and gas production emissions data for outside of the WRAP region are contained in the stationary-area inventories.

2.10.2 Emissions Processing

We modeled the WRAP point-source oil and gas production emissions in combination with the rest of the stationary-point-source emissions. We modeled the WRAP area-source oil and gas production emissions explicitly as a separate category that included WRAP and tribal inventories. These data represent weekly average emissions and did not require any renormalization within SMOKE. We used spatial surrogates generated by ENVIRON to allocate these annual county-level emissions to the model grid. For all oil and gas emissions, we applied flat temporal profiles to create hourly inputs to CMAQ and CAMx.

2.10.3 Uncertainties and Recommendations

In future 2002 modeling California oil and gas production emissions should be replaced with revised data provided by the California Air Resources Board (CARB). In addition, WRAP has

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updated their oil and gas production inventory for the base and future years in a Phase II work effort that substantially improved the emissions inventory estimates (Bar-Ilan et al., 2007).

2.11 MMS Off-shore Gulf of Mexico Emissions

Offshore area point source emissions include emissions in the Gulf of Mexico and off the coast of California that are associated with oil and gas drilling platforms.

2.11.1 Data Sources

We obtained year 2000 IDA-formatted point-source inventories for oil and gas platforms in the Gulf of Mexico from the Minerals Management Service (MMS) web site:

http://www.gomr.mms.gov/homepg/regulate/environ/airquality/gulfwide_emission_inventory/2000GulfwideEmissionInventory.html

We combined these with point-source data for coastal California provided to us by CARB during the preliminary 2002 modeling. We also obtained gridded area source emissions for platforms in the Gulf of Mexico from the MMS that we converted to the CENRAP 36-km model grid.

The 2000 MMS Gulf wide Emission Inventory was updated as of June 2006 to account for a change in vessel emissions in the non-point source (non-platform) database file. The point source (platform) emission inventory database file has not changed from the original version. Area source emissions from offshore activities in the Gulf of Mexico were developed from the latest estimates provided by the Minerals Management Service (MMS). The MMS inventory includes both platform and non-platform sources. The non-platform area source emissions estimates are spatially allocated to lease blocks and protraction units throughout the Gulf of Mexico. Temporal and spatial allocation cross-reference data were developed from the MMS inventory data and formatted for input to the SMOKE emissions model by Carolina Environmental Programs. These data were provided to the CENRAP emissions modeling team for implementation within SMOKE. The spatial allocation surrogates were provided for 4-km grid cells. The UCR team used these surrogates and developed surrogates for 36-km grid cells. Because these data are references to lease blocks/protraction units, rather than counties, this source category was processed separately from all other emissions using a customized reference data and SMOKE run scripts.

We modeled the offshore point and area sources as separate categories in the simulations. We used SMOKE to locate the offshore point sources on the model grid and to vertically allocate them into 15 model layers.

To QA the offshore platform emissions, we used the procedures in the CENRAP modeling QAPP (Morris and Tonnesen, 2004) and Modeling Protocol (Morris et al., 20042) and a suite of graphical summaries. We used tabulated summaries of the input data and SMOKE script settings to document the data and configuration of SMOKE for simulation Base02a. The graphical QA summaries include, for all emissions output species, daily spatial plots, daily time-series plots, and annual time-series plots. These QA graphics are available at <http://pah.cert.ucr.edu/aqm/cenrap/index.shtml> for the point and area sources.

2.11.3 Uncertainties and Recommendations

While the MMS data that we used were an improvement over previously modeled Gulf of Mexico platform inventories, the data were developed for a different modeling application that covered only the extreme northwestern portion of the Gulf, so they are missing large areas of the region of the Gulf that contain drilling platforms. The California offshore inventory represents an initial attempt at compiling an emission inventory for this area and contains very few sources. Future simulations will focus on improving these emissions by expanding the coverage of the offshore platform inventories for both the Gulf of Mexico and the Pacific Coast.

2.12 Off-shore Shipping Emissions

Emission inventory development for regional- and continental-scale air quality modeling has historically neglected offshore emissions sources beyond 25 miles offshore. Concern over the environmental effects of commercial shipping emissions in the Pacific on the coastal states in the WRAP region led to the development of a commercial marine shipping inventory for the Pacific. This inventory of off-shore marine vessels emissions made a substantial difference in some of the coastal western PM estimates (e.g., SO₄). VISTAS developed an off-shore marine vessels inventory for the entire modeling domain that included the Pacific and Atlantic Oceans and the Gulf Of Mexico. For Typ02G and Base18G emission inventories CENRAP adopted the offshore shipping inventories developed by VISTAS.

2.12.1 Data Sources

Initially we obtained gridded annual commercial marine shipping emissions for the Pacific on the 36-km model grid from WRAP for inclusion in CENRAP simulations in the Base F modeling (Pollack et al., 2006). The commercial marine inventory contains all of the criteria pollutants contained in the non-road mobile-source inventory: CO, NO_x, VOC, NH₃, SO₂, PM₁₀, and PM_{2.5}. This inventory was subsequently updated in the Typ02G and Base18G modeling with the VISTAS off-shore commercial marine emissions inventory that covered the Gulf of Mexico and the Atlantic and Pacific Oceans and was based on the EPA/ARB SO_x Emissions Control Area (SECA) program. Dr. James Corbett (University of Delaware) analyzed off-shore marine vessel data and worked with ENVIRON/ICF to convert to gridded emissions for the SECA grid. ENVIRON then provided SO₂, NO_x, PM and VOC emissions for the RPO 36-km grid.

2.12.2 Emissions Processing

The commercial marine shipping inventory was not processed through SMOKE. VISTAS provided the data to the as gridded text files on the 36-km model grid. These data were reformatted to the NetCDF CMAQ input format with a utility developed by UCR. The VOC inventory was converted to CB-IV speciation and the NO_x and PM_{2.5} inventory pollutants to CMAQ input species with SMOKE chemical profiles for commercial shipping sources. No temporal adjustments were applied to these emissions; they use uniform monthly, daily, and diurnal profiles. An SCC for commercial marine vessels within the MMS inventory (SCC CM80002200) was accounted for in the commercial marine inventory developed for VISTAS.

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The duplicate emissions were removed from the MMS inventory prior to processing emissions for Base G simulations. The duplicated emissions amounted to 19,000 TPY of NO_x and 3,184 TPY of SO₂. For simulation Typ02G and Base18G we received binary netCDF file from ENVIRON for one day and that day was used for every day of the year.

To QA the commercial marine shipping emissions, we used the procedures in the CENRAP modeling QAPP (Morris and Tonnesen, 2004) and Modeling Protocol (Morris et al., 2004a) and a suite of graphical summaries. The graphical QA summaries include, for all emissions output species, daily spatial plots, daily time-series plots, and annual time-series plots. These QA graphics are available at <http://pah.cert.ucr.edu/aqm/cenrap/index.shtml>.

2.12.3 Uncertainties and Recommendations

As a first attempt at representing shipping emissions in the Pacific in international waters, the WRAP and VISTAS 2002 commercial shipping inventory is a breakthrough in a historically neglected emissions category. As the RPOs evaluate the effects of these emissions on the air quality modeling, we anticipate that there will be refinements to the temporal profiles and to the vertical allocation of the emissions. Many of the stacks of large commercial ships contained in this inventory extend vertically above the first model layer. Future versions of this inventory should use higher-resolution temporal adjustments and should allocate the emissions to the appropriate model layers. Off-shore marine shipping activity is projected to increase. However, there are also the potential for emission controls on this source category (e.g., SECA program). Given these two off setting activities, the 2002 off-shore marine shipping emissions were assumed to be unchanged going from 2002 to 2018. Better estimates of 2018 marine emissions are being developed that should be considered in future modeling activities.

2.13 2018 Growth and Control

Base18G was based on grown inventories assuming on-the-books control strategies. CENRAP contracted with Pechan to deliver growth and control data for CENRAP and to consolidate growth and control information for other RPOs where available (Pechan, 2005d). The data are applicable to all source categories and pollutants included in the CENRAP 2002 emission inventory. This includes the following pollutants: sulfur oxides (SO_x), oxides of nitrogen (NO_x), volatile organic compounds (VOC), carbon monoxide (CO), ammonia (NH₃), and primary PM₁₀ and PM_{2.5}. Some source categories were held constant between 2002 and 2018 because either stagnant growth was deemed appropriate or insufficient data was available to adequately project future growth or controls. These source categories include the following:

- Wind Blown Dust from non-agricultural land use categories.
- Emissions from wildfires.
- Emissions from Mexico.
- Global transport sources (i.e., the 2002 GEOS-CHEM boundary conditions).

2.13.1 Data Sources

CENRAP contracted with Pechan to provide growth and control factors to be applied with SMOKE for the CENRAP region (Pechan, 2005d). These growth and control parameters were

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based on growth estimates derived from EGAS 5.0 and control estimates assumed for implementation of federal regulations and on-the-books state and local control programs. Emissions projections for electric generating units were developed for the RPOs with the Integrated Planning Model (IPM). The RPO 2.1.9 IPM results were subsequently modified by VISTAS, MRPO and CENRAP to reflect planned new construction and controls. The WRAP provided 2018 EGU estimates developed in coordination with State and Industry stakeholders. VISTAS, MWRPO and the WRAP provided emissions for 2018, having applied growth and control factors outside of SMOKE processing. EPA provided SMOKE processed emissions, applying both growth and controls, for Canada for the year 2020. These emissions were provided on the RPO 36-km grid. However, emissions were inexplicably processed for an alternative vertical structure. Alpine Geophysics, under contract to VISTAS reallocated the emissions through the vertical layers to more accurately reflect the vertical structure applied uniformly by the RPOs. The modified data was obtained directly from Alpine Geophysics. Emissions from Mexico were held constant between the inventory year 1999 and modeled 2002 and 2018. Improvements to the Mexican inventory have been continuously made between generation of the original BRAVO inventory and the present improved 1999 inventory. However, given the continued uncertainties in the improved inventory, no future year projections were attempted by CENRAP.

2.13.2 Emissions Processing

Growth and control factors developed by Pechan (2005d) for Arkansas did not match the final delivered inventory for Arkansas. Arkansas underwent major revisions to point and facility IDs in mid-2005. These updates were not available by the delivery date of the growth and control parameters. In coordination with Arkansas, a cross-walk was developed to correct the point and facility IDs.

The assumptions that went into the development of controls for engines covered under the RICE MACT were not consistent with the final rule. Rule penetration values for CENRAP states were adjusted to more accurately reflect the impact of the final rule.

The impact of the refinery global settlements was not incorporated into CENRAP modeling until the base G simulations. Control assumptions provided by EPA and referenced in EPA CAIR modeling were applied to the 2018 inventory. These reductions primarily impacted SO₂ emissions; however, NO_x reductions were applied in Oklahoma, Louisiana, and Minnesota.

2.13.3 Uncertainties and Recommendations

The impact of control programs is an area of uncertainty that will need continued review as the programs are implemented. Development of growth and control assumptions for Mexico will be necessary for continued refinement of the impact of international transport. CENRAP obtained estimates of increased prescribed burn activity for the Forest Service after processing of the base G simulations was underway. These estimates of increased activity should be reviewed for inclusion in future simulations. EPA developed 2020 estimates of Canadian emissions are assumed to include erroneous stack parameters previously addressed in the 2000 emissions processing. Further review of this data set is recommended.

2.14 Emissions Summaries

Appendix B provides details on the source of the emission files used in the CENRAP Typ02G and Base18G modeling. Also in Appendix B are sample emission summary plots, additional plots are available on the CENREAP modeling website:

<http://pah.cert.ucr.edu/aqm/cenrap/emissions.shtml>.

CENRAP has contracted with E.H. Pechan and Associates to provide emissions summaries used in the final Typ02G and Base18G modeling in Excel spreadsheets and in an Access database that are available on the CENRAP website (<http://www.cenrap.org/projects.asp#>). Figures 2-3 through 2-9 display the, respectively, SO₂, NO_x, VOC, PM_{2.5}, PM₁₀, NH₃ and CO anthropogenic emissions for the CENRAP states and the Typ02G and Base18G emission scenarios. Emissions are broken down by major source sector. For the state of Texas the emissions are broken by three groups, northeast Texas, southeast Texas and remainder of Texas (west Texas).

For most states, EGUs are the largest contributor to SO₂ emissions (Figure 2-3). As EGU SO₂ emissions are generally projected to be reduced in the future, most states show a reduction in total SO₂ emissions from 2002 to 2018. One exception to this is Louisiana for which non-EGU point source SO₂ emissions are greater than for EGU and are projected to increase from 2002 to 2018. The reasons for these increases are unclear, but the growth factors for non-EGU points should be examined more carefully.

NO_x emissions are fairly evenly distributed across non-EGU point, EGU point, non-road mobile, on-road mobile and area sources for the 2002 Typ02G emissions scenario (Figure 2-4). In 2018, the contributions of on-road mobile source NO_x emissions is reduced dramatically, with some states also showing reductions in EGU NO_x emissions as well, resulting in all states exhibiting lower NO_x emissions in 2018 than 2002.

VOC emissions are dominated by area, non-road mobile, on-road mobile and non-EGU point sources in both 2002 and 2018 (Figure 2-5). VOC emissions from on-road and non-road mobile source are projected to go down in the future, whereas VOC emissions from non-EGU point and, especially, area sources are projected to increase. Thus, whether a state's total VOC emissions increase or decrease depends on the relative contributions of mobile versus area sources and the level of increase in area source VOC emissions. Note that the VOC emissions listed in Figure 2-5 do not include biogenic VOC emissions that would be greater than the anthropogenic VOC emissions shown in Figure 2-5. Note that because biogenic VOC emissions are processed using the SMOKE/BEIS module on the 36 km grid, state-wide biogenic VOC emissions summaries are not readily available.

Primary PM_{2.5} emissions are primarily from road dust and fugitive dust, and for some states fires (Figure 2-6). Kansas, Oklahoma, Louisiana and Texas all have large contributions from fires not seen in the other states. Road dust and fugitive dust are the most dominate source categories for coarse particulate as well (Figure 2-7).

CENRAP developed a separate ammonia emissions for 13 categories using the CMU model including livestock and fertilizer that dominates the ammonia emissions across the CENRAP

states (Figure 2-8). Several states also have significant ammonia contributions from non-EGU point sources, whereas others do not.

CO emissions are dominated by the on-road and non-road mobile source sectors (Figure 2-9). However, states with fires also see large CO contributions from them as well. On-road mobile source CO emissions are projected to go down substantially from 2002 to 2018, whereas the other source categories are flat.

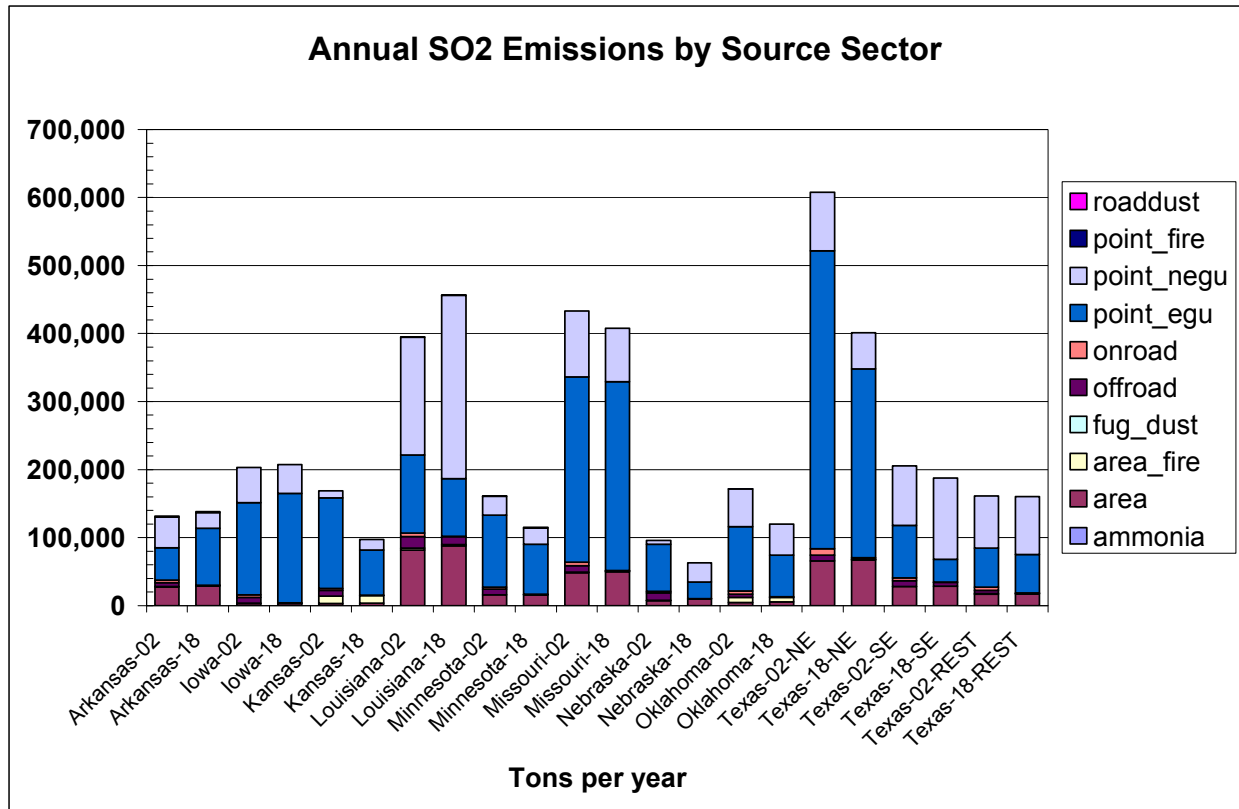


Figure 2-3. Summary of Typ02G and Base18G SO2 emissions by CENRAP state and major source sector (tons per year).

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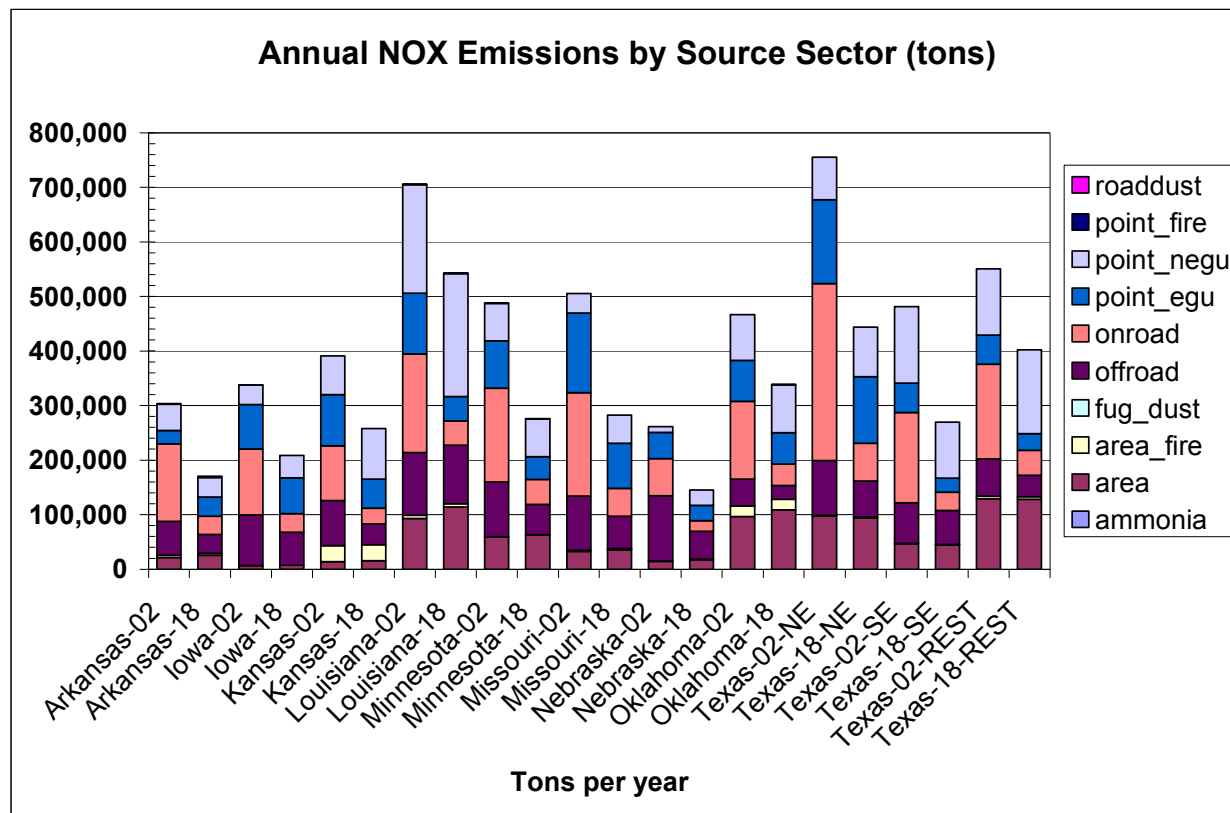


Figure 2-4. Summary of Typ02G and Base18G NOx emissions by CENRAP state and major source sector (tons per year).

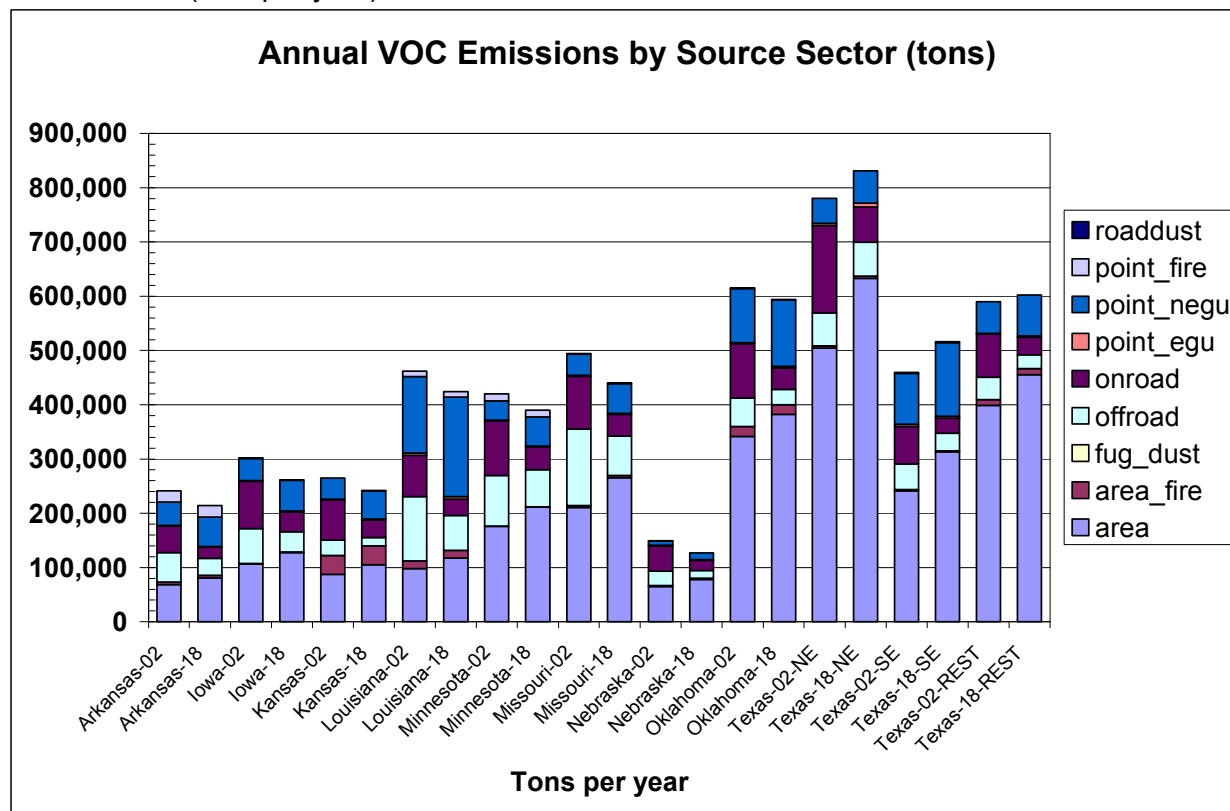


Figure 2-5. Summary of Typ02G and Base18G VOC emissions by CENRAP state and major source sector (tons per year).

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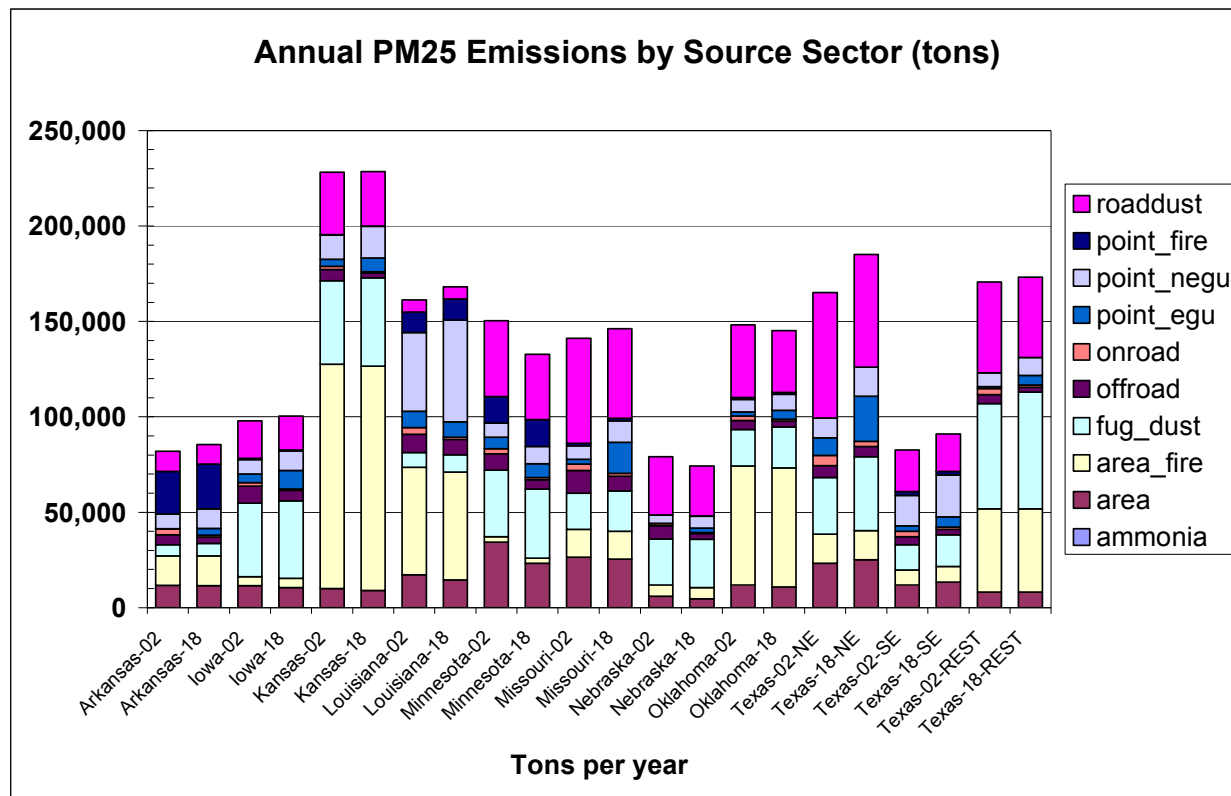


Figure 2-6. Summary of Typ02G and Base18G PM2.5 emissions by CENRAP state and major source sector (tons per year).

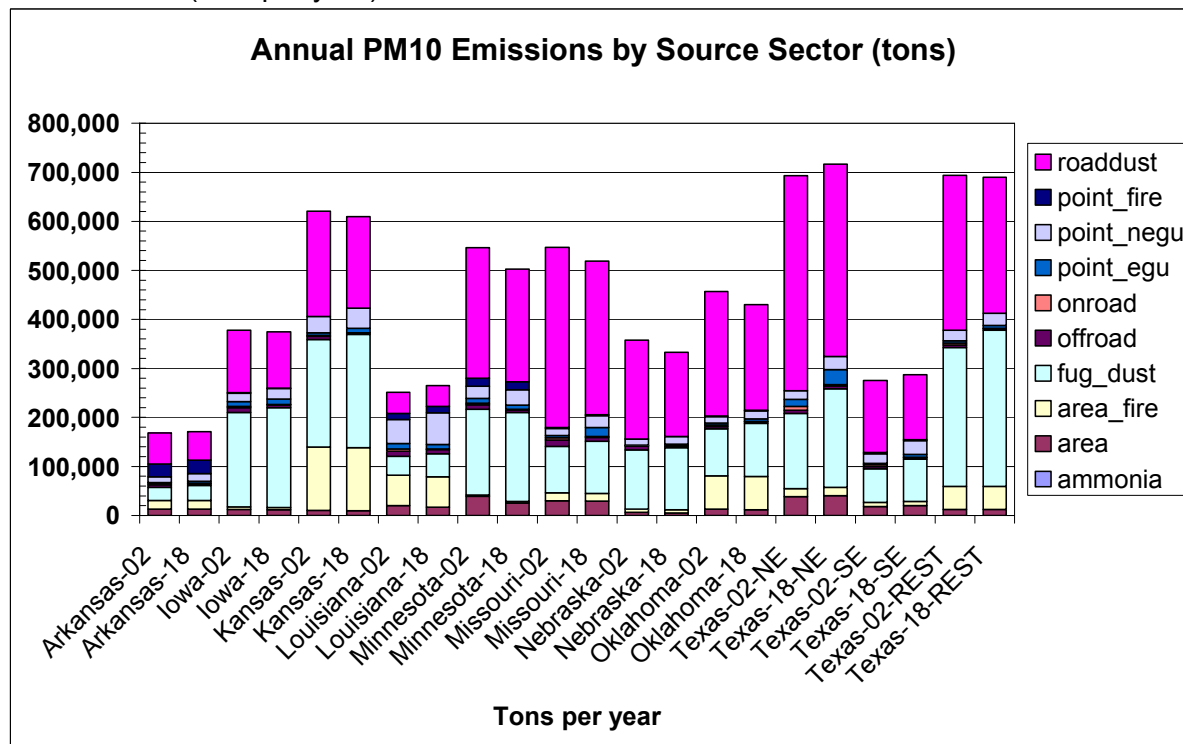


Figure 2-7. Summary of Typ02G and Base18G PM10 emissions by CENRAP state and major source sector (tons per year).

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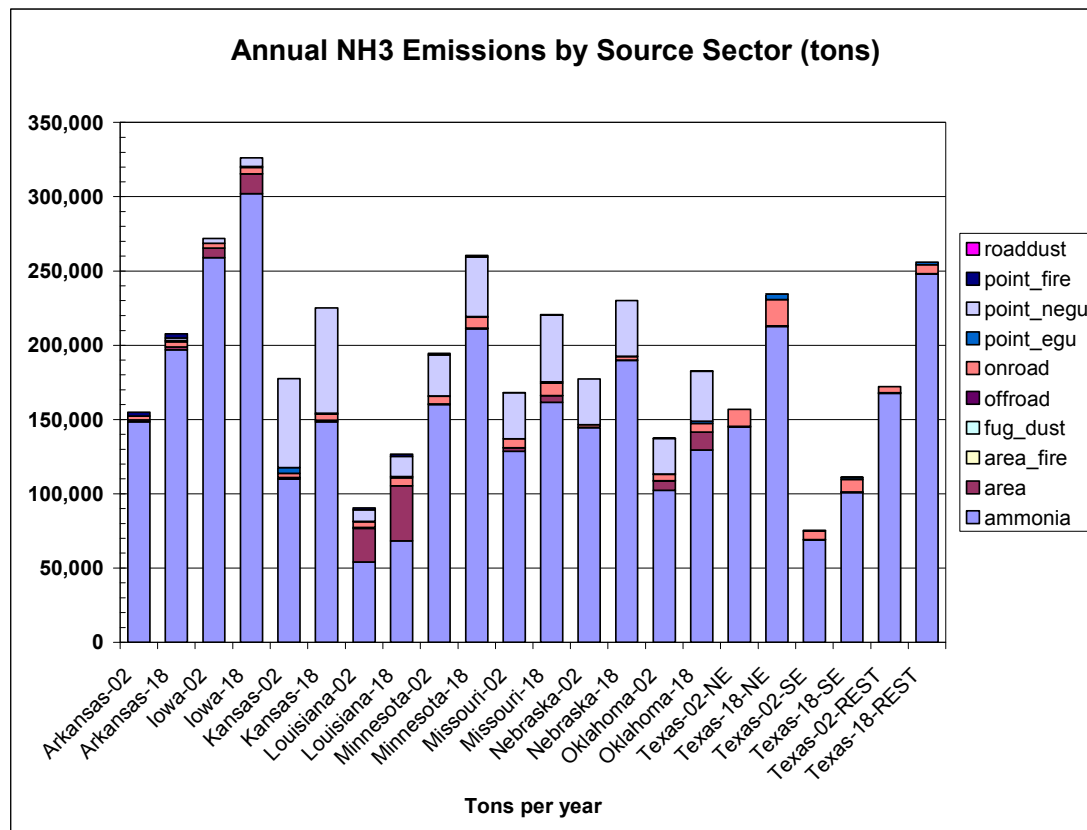


Figure 2-8. Summary of Typ02G and Base18G NH3 emissions by CENRAP state and major source sector (tons per year).

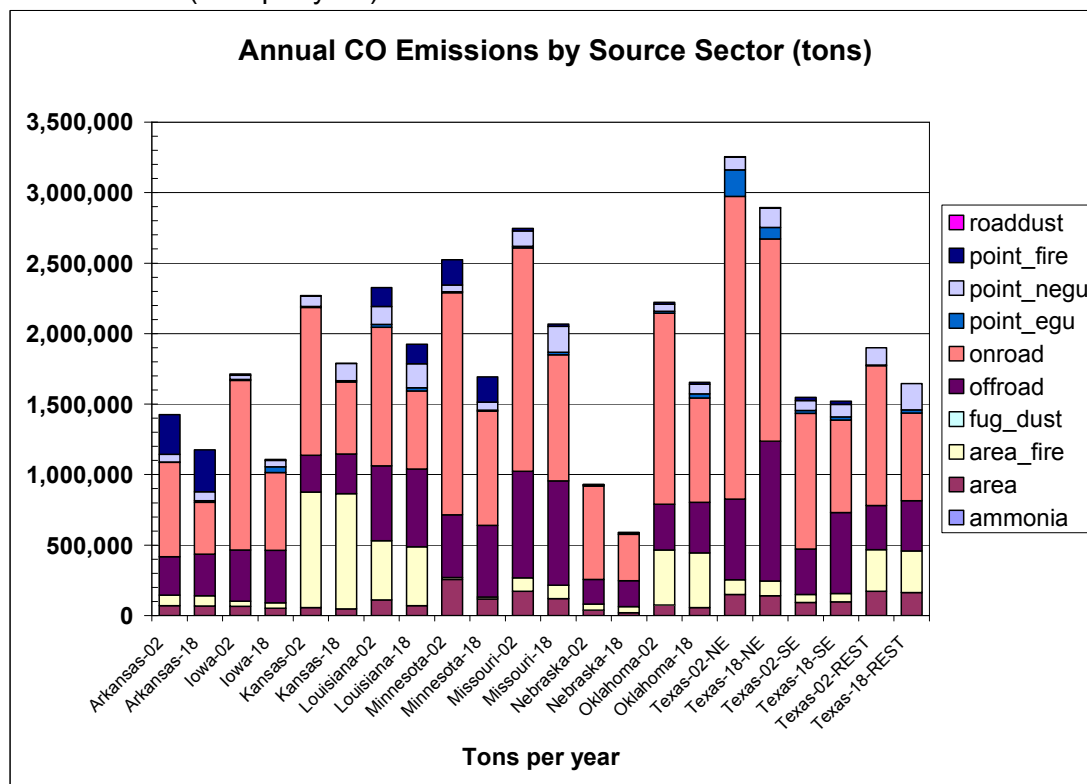


Figure 2-9. Summary of Typ02G and Base18G CO emissions by CENRAP state and major source sector (tons per year).